The Stochastic Human Exposure and Dose Simulation Model for Multimedia, Multipathway Chemicals (SHEDS-Multimedia):Residential Module

SHEDS-Residential version 4

Draft User Guide

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Acknowledgements

We would like to thank our colleagues in EPA's Office of Pesticide Programs, and Dr. Andrew Geller in EPA's Office of Research and Development, for their review of this User Guide.

Computing Issues, Disclaimer, and Support

Computing Issues
It is strongly advised that the SHEDS user maximize windows so that as much as possible of the full dialog is displayed. You may still need to scroll down to see all of some dialogs. Refer to the images in this User Guide to ensure that all components of a dialog are displayed.

It is highly recommended that the user pause or disable any automated anti-virus or back-up programs that access the SHEDS installation or data output directories, or place these directories in locations that are not virus-checked or backed up. Such programs may access SHEDS data files and interfere with model performance, causing unpredictable results.

Disclaimer
EPA's SHEDS-Residential version 4 model can simulate cumulative (multiple chemicals) or aggregate (single chemical) residential exposures over time via multiple routes of exposure for different types of chemicals and scenarios. The United States Environmental Protection Agency, through its Office of Research and Development, developed and funded SHEDS-Residential version 4 with assistance from contractor Alion Science and Technology, Inc.

SHEDS-Residential version 4 is one module (along with the separate SHEDS-Dietary module) of EPA's more comprehensive human exposure model, the Stochastic Human Exposure and Dose Simulation model for multimedia, multipathway chemicals (SHEDS-Multimedia), which can simulate aggregate or cumulative exposures over time via multiple routes of exposure (dietary & non-dietary) for different types of chemicals and scenarios. SHEDS-Residential and SHEDS-Dietary will be merged together in a future version of SHEDS-Multimedia.

SHEDS-Residential version 4 includes a case study example for illustrative purposes, as well as a default file for non-chemical specific inputs, as described in the Technical Manual and User Guide. All input values used in the SHEDS-Residential model for a given application should be entered or reviewed by the researcher so that the model results are based on appropriate data sources for the given application.

Version 4 of SHEDS-Residential reflects comments from EPA's August 2007 external Scientific Advisory Panel that reviewed SHEDS-Multimedia version 3 (the aggregate residential version). SHEDS-Residential version 4 will undergo external peer review by EPA's Scientific Advisory Panel July, 2010, and should be considered draft at this time.

Support
Please contact one of the following individuals with any questions, comments, or specific suggestions related to this beta version of the SHEDS model:

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ACRONYMS AND ABBREVIATIONS

CDFs – cumulative distribution functions
CHAD – Consolidated Human Activity Database
EPA – United States Environmental Protection Agency
GI – gastrointestinal
GM – geometric mean
GSD – geometric standard deviation
GUI – graphical user interface
NERL – National Exposure Research Laboratory
NOAEL – no observed adverse effect level
ORD –Office of Research and Development
PBPK – physiologically-based pharmacokinetic
PDFs – probability density functions
SHEDS – Stochastic Human Exposure and Dose Simulation
ug (in SAS printout or variable names) – microgram

1 Considerations for New Users of SHEDS-Residential

1.1 Introduction

SHEDS-Residential version 4 (also referred to in this user guide as 'SHEDS') is a sophisticated but user-friendly cumulative and aggregate human exposure model for chemicals contacted in a residential setting. It requires the user to select appropriate inputs and to interpret the resulting outputs. Users should therefore be prepared to invest time to configure this model to exposure scenario(s) of their choice. Before attempting to run the model, it is recommended that new users review this User Guide and the Technical Manual to familiarize themselves with the model and the types of information that will be required.

The SHEDS installation package includes the User Guide, Technical Manual, annotated SAS code for use via the graphical user interface (GUI), Consolidated Human Activity Database (CHAD) activity diary and population files, a height/weight data set, and default input distributions. The installation process is explained in this User Guide, which is intended to guide the user through the GUI. The interface has three functions: specifying inputs, executing the model, and storing and viewing the results. The Technical Manual contains a detailed description of the model's structure and algorithms.

The SHEDS model runs on a personal computer and requires that SAS 9.1 or higher be installed prior to the installation of SHEDS. It has been run successfully on various laptops and desktops using Windows XP. It has not yet been tested with Windows Vista. Though hardware requirements are modest, a full-scale model run may take a substantial amount of time. As a rough guide, a variability-only (1-stage Monte Carlo) run takes about 1 hour for every 1000 persons being simulated and a typical run may be several thousand persons. Uncertainty (2-stage Monte Carlo) runs are much slower and may take several days to complete.

SHEDS is a stochastic model in which each simulated individual is different. There are approximately 100 variables that can be sampled randomly for each person (although not all of these variables apply for a given model simulation); many of these variables require multiple samples per person as they change over time throughout the simulation period. Increasing the number of simulated individuals provides a better characterization of the population under study.

SHEDS separately constructs time series for the environmental concentrations in each simulated person's house, as well as an activity sequence through time based on the selection of human activity diaries from EPA's Consolidated Human Activity Database (CHAD; http://www.epa.gov/chadnet1). These are combined, using exposure pathway-specific equations and exposure factors sampled from user-specified distributions, to generate a time series of exposure for each simulated individual. The time step is variable and depends on the event duration from the activity diaries, ranging from one minute to one hour. Therefore, a 1-year

simulation will have a very large number of such events (generally 10,000 to 20,000) for each simulated person. These results are automatically aggregated over time to produce (for example) daily exposure totals, although for some purposes the finer time resolution may be useful. Due to their size, the event-level exposure time series are not usually saved as permanent output; as a rule only summary statistics on daily and longer periods are saved.

SHEDS does not attempt to model the exposures of particular individuals. Instead it randomly creates a population of simulated individuals who collectively represent the target population. Thus, an appropriate result of a model run might be the statement 'SHEDS indicates that 5% of the target population receives an exposure in excess of …', but it is not appropriate to say that a specific real-world individual receives any particular exposure.

SHEDS has a graphical user interface (GUI) that guides the user through the various input screens. The GUI comes with a demonstration scenario. It may be useful to copy this under a new name and to make changes to this copy. This is described in more detail later in this manual.

SHEDS version 4 allows consideration of multiple chemicals per model run. The user may also select several scenario categories (each containing one or more of the different chemicals) to be analyzed together in the same run. The model permits the use of co-occurrence factors that control the likelihood of the various scenarios being applied at the same house at the same time. The human exposure results are automatically aggregated across the scenarios used in the given model run. The cumulative exposure results for all chemicals in the simulation are also determined.

1.2 Entering Distributions

Many SHEDS inputs are randomly sampled from user-specified distributions. SHEDS accepts a wide variety of continuous distributions as detailed in Appendix C. Some inputs require probability vectors (see the Appendix and section 4.1.1 of the Technical Manual). For continuous distributions, the user selects the type from a pull-down menu and then specifies the desired parameters. For discrete distributions (probability vectors) the user enters the probability of each outcome.

The GUI will highlight invalid choices with a yellow background. This usually results from numeric parameters being specified that are incompatible with the type of distribution. For example, the lognormal distribution requires a geometric mean greater than zero and a geometric standard deviation greater than one. A missing numeric parameter will also result in the yellow error indicator. For probability vectors, the sum of the probabilities must be one or else an error will be indicated.

The user has the option of truncating distributions at one or both ends by specifying minimum and/or maximum values. If the random number generation produces values outside these limits

then the values are automatically reset to the maximum or minimum, depending on which was exceeded.

1.3 Configuring SHEDS to the Scenarios of Interest

The user has the ability and the responsibility to configure SHEDS to a particular scenario(s) of interest. This includes specifying the target population, the simulation period, the chemical and application method(s) of interest, and the distributions for many model parameters. As an example, SHEDS supports three methods of determining the chemical concentrations: user-supplied time series, a decay/dispersion model based on chemical application dates, or a post-application decrease based on time intervals. The user must choose which one is most appropriate for the problem at hand. These three methods are described in more detail in the SHEDS Technical Manual.

The SHEDS installation package comes with example input distributions for demonstration purposes, to help orient users in how to run the model. These values can be used as a starting point for becoming familiar with the GUI, or modified by the user as appropriate.

SHEDS is designed to estimate human exposure in a residential setting, but is not geared to any specific chemical. The user customizes the model run for the chemical of interest by setting appropriate input parameters, for example, product types and usage frequencies, initial application amounts, and concentration decay rates. The model allows the user to select one or more scenario application methods from a pre-determined list in the GUI.

The SHEDS GUI allows the user to select the gender and age range of the target population. Again, SHEDS is a population-based model; therefore it would be appropriate for simulating exposure for school-age children in general, for example, but should not be expected to be reliable for simulating a specific child or even a specific set of children. Beyond age and gender, the user may target populations by selecting input distributions that reflect characteristics of those groups.

SHEDS follows the real-world calendar. The "simulation period" is the user-specified time over which the exposure is tracked for each simulated individual. The model allows this to range from one day to several years, but the user should be aware of certain considerations. For example, if the user supplies concentration time-series data, then the period is limited to the extent of this data. Note that SHEDS version 4 does not change the age of individuals within the simulation period, and therefore simulation periods longer than one year may not be advisable for children. Finally, longer simulations require longer run times.

SHEDS calculates exposure from several different pathways. If desired, the user may restrict the model to selected pathways by judicious specification of inputs. For example, ingestion of chemical via object mouthing can be "turned off" simply by setting the distribution for object-to-mouth contact frequency to a point value of zero. Similarly, other pathways such as inhalation, hand mouthing, direct soil ingestion, dermal absorption, and GI tract absorption could be turned off.

There is no facility to supply differing inputs by region within a single run in SHEDS version 4. To model regional variation the user would have to construct a separate model run for each region with distinct input distributions. The distributions for each run would then reflect the variation within the given region (but not across regions). For example, pesticide usage may differ in warm and cold climates. Seasonal variation in pesticide usage is built into the model, as is seasonal variation in the human activity diaries. However, other inputs are assumed not to have seasonal variation when input via the GUI. By bypassing the GUI, advanced SAS users have the option of incorporating seasonal variation in distributions within a single model run.

2 Overview

2.1 Introduction

Reliable models for assessing human exposures are important for understanding health risks from chemicals. The Stochastic Human Exposure and Dose Simulation model for multimedia, multiroute/pathway chemicals (SHEDS-Multimedia), developed by EPA's Office of Research and Development (ORD), National Exposure Research Laboratory (NERL), is a state-of-science computer model for improving estimates of aggregate (single-chemical, multi-route/pathway) and cumulative (multi-chemical, multi-route/pathway) human exposure and dose. SHEDS-Multimedia is the EPA/ORD's principal model for simulating human exposures to a variety of multimedia, multipathway environmental chemicals such as pesticides, metals, and persistent bioaccumulative toxins. Exposure is defined in SHEDS-Multimedia as the contact between a chemical agent and a simulated human target at the external surfaces (skin and oral/nasal passage). Dose is defined in SHEDS-Multimedia as the amount of chemical that enters the target after crossing the exposure surfaces. As stated in section 1.1, SHEDS-Multimedia version 4 is comprised of both a residential module (SHEDS-Residential version 4.0), described in this user guide and a related technical manual (Glen et al., 2010), and a dietary module (SHEDS-Dietary version 1.0; Xue et al., 2010; Isaacs et al., 2010). This user guide focuses on the SHEDS-Residential version 4.0 module only. However, please note that in anticipation of merging the residential and dietary modules in SHEDS-Multimedia, the name "SHEDS-Multimedia" appears on some of the screenshots in this user guide rather than "SHEDS-Residential."

SHEDS-Residential is a physically-based, probabilistic model that predicts, for user-specified population cohorts, exposures incurred via inhaling contaminated air, touching contaminated surface residues, and ingesting residues from hand- or object- to-mouth activities. To do this, it combines information on chemical usage, human activity data (e.g., from time/activity diary surveys and videography studies), environmental residues and concentrations, and exposure factors to generate time series of exposure for simulated individuals. One-stage or two-stage Monte Carlo simulation is used to produce distributions of exposure for various population cohorts (e.g., age/gender groups) that reflect the variability and/or uncertainty in the input variables. While the core of SHEDS-Residential is the concentration-to-exposure module, there are various options (built-in source-to-concentration module; user-entered time series from other models or field study measurements) for obtaining concentration inputs and dose outputs (SHEDS-Residential has a built-in simple pharmacokinetic (PK) model, and SHEDS-Residential exposure outputs can be used as inputs to physiologically-based pharmacokinetic (PBPK) models).

For a more detailed technical description of the SHEDS model, please refer to the SHEDS-Residential version 4 Technical Manual. The purpose of this User Guide is to assist the SHEDS-Residential user in navigating through the graphical user interface to apply SHEDS-Residential. Figure 2.1 provides an overview of the SHEDS-Residential user interface. Differences between the Version 3 interface and Version 4 are noted. The major interface screens are each represented with one box; not all screens are represented in Figure 2.1 (page 8). In general, the

user will navigate through the interface from left to right and top to bottom as shown on the overview. The exact screens visited will vary depending on the type of run being defined and data required for that run. Typically, the interface will prevent the user from moving ahead unless all data for the current step have been entered.

The user interface guides the user through a set of screens that define the inputs needed for a SHEDS run. When a new run is created, most of these screens contain default choices, or choices from a previous model run, that the user may either edit or accept. The best way to run SHEDS is to carefully prepare the inputs for an initial baseline run; thereafter, one can start with the baseline run and make a small number of changes from run to run, greatly speeding up the process. A default file for non-chemical specific inputs is included with SHEDS-Residential version 4 (see Appendix G of the Technical Manual); these can be used for a simulation or modified by the user.

Some sections will need to be revisited a number of times to enter all information. In particular, the sections defining application details and dates, and those defining media concentrations will need to be defined for each application or scenario type being simulated. The screens used to enter variability distributions will need to be revisited for each group of variables being defined.

Every effort has been made to reduce the amount of information entered by the user. For instance, if dermal transfer efficiencies are being used, then the user will not be presented with the opportunity to enter data on dermal transfer coefficients. Likewise, if the decay and dispersion module is being used to model media concentrations, users will only enter information relevant to that and not to time-series or interval distributions.

2.2 Using the Demonstration Case Study for Permethrin

When installed, SHEDS-Residential version 4 comes with a completed sample run. This sample run is named “Permethrin Case Study” and is meant to assist the user in becoming familiar with the interface. This Case Study simulates a single scenario: a crack-crevice aerosol containing Permethrin. The simulations last one year for each individual, use the decay and dispersion method for simulating concentrations, use transfer efficiencies rather than transfer coefficients for dermal exposure calculations, and use the longitudinal diary assembly method. The run supplied contains results for 500 people. The user may change this value and re-run the simulation if a different number is desired. A typical production run will require substantially more individuals. Chapter 6 of the manual instructs the user how to re-create this run from scratch.

The results from the file are available on installation and can be viewed by selecting the View Results of Selected Run button on the Specify Run Name dialog (described on page 26). While the inputs in the Permethrin Case Study will not be changed when you use the View Results button, changes made after selecting the file with Edit Selected Run will overwrite the original values. **It is strongly recommended that the user not edit the original Permethrin Case Study**. To view and edit inputs from the demonstration, go to the Specify Run Name dialog (described on page 26), highlight “Permethrin Case Study”, and click on Copy Selected Run To

New Run. You will be prompted for a new run name. After entering the run name and visiting the Run Files screen you will be free to make any desired changes without affecting the original Permethrin Case Study.

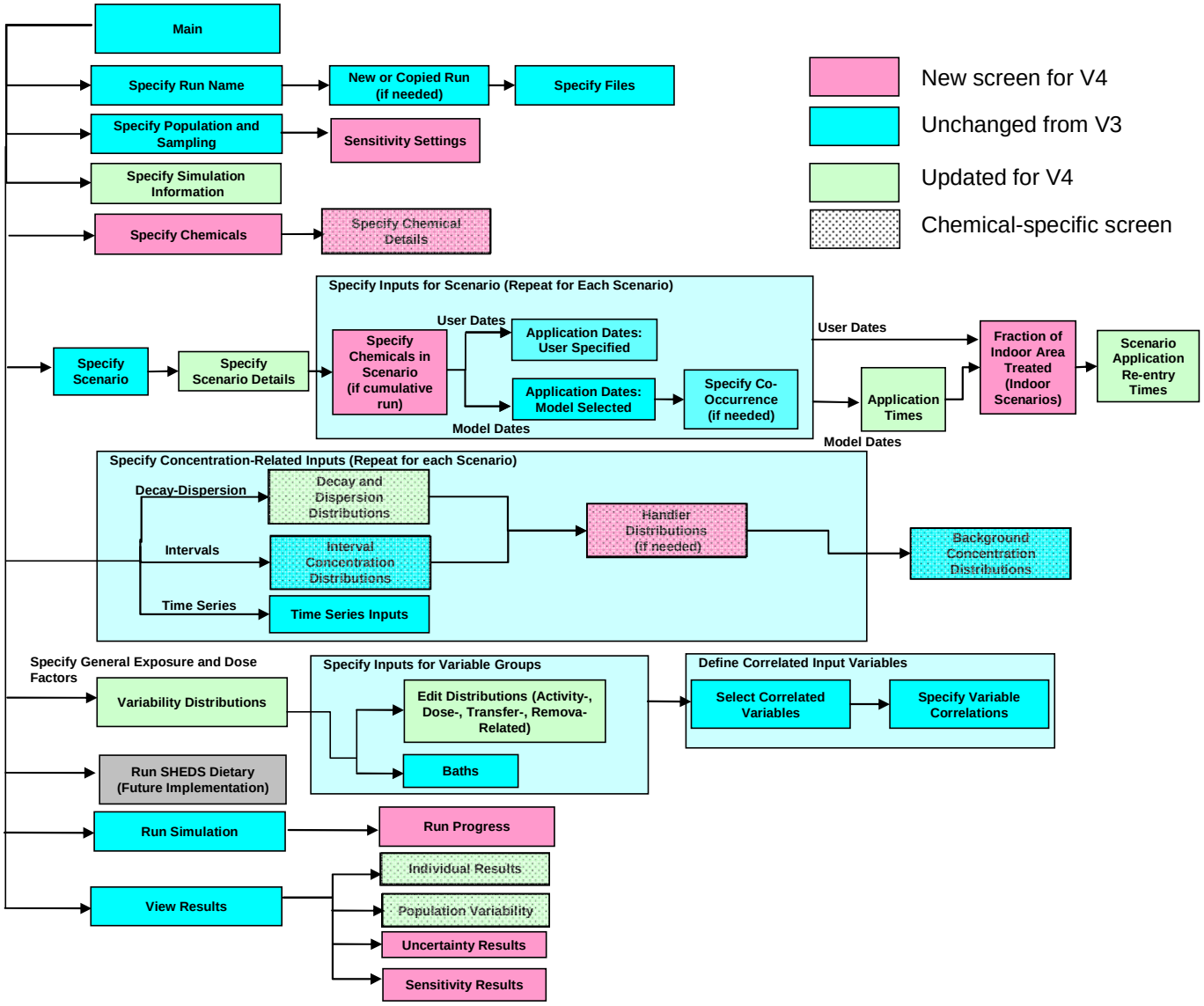


Figure 2.1. Overview of the SHEDS-Residential Interface at Version 4.

2.3 General Interface Hints

2.3.1 Display Issues

Display issues can arise when SAS does not have room to display the entire dialog. When a screen does not initially draw correctly, either the top title text or the bottom left button (Continue, or Return) do not display. If in doubt, compare the display to the appropriate figure in this manual. The easiest method of minimizing these issues is to maximize the main SAS window. On smaller monitors some screens may still not display fully. The screen's scroll bars should be used to view the bottom of the screen. Unfortunately, SAS does not always display the scroll bars automatically. Resizing the SHEDS dialog will force SAS to redraw the dialog and include scroll bars if necessary.

Figure 2.2. Example of List Box with a Blue Background Indicating There are More Groups to Complete.

2.3.2 Grayed Out Buttons or Widgets

Occasionally buttons will be grayed out (displayed with muted text, see Figure 2.3). This may mean that a function has not been implemented. In version 4 the Help and About buttons have not been implemented yet.

Figure 2.3. Sample of Two Buttons, One Normal and One Grayed Out (Bottom).

In many cases a grayed out button means that additional steps are required before the user is permitted to enter certain data. This is particularly true on the main screen where data entry must be completed sequentially, by starting at the top button and working down. There are also several screens where the user must complete data entry or editing for each group of variables listed before continuing. In these cases, the groups are listed on the left and all completed groups are listed on the right. If the groups remain uncompleted, the completed list is highlighted in a light blue (Figure 2.2). Another reason a button may be grayed out (Figure 2.3) is due to a current error on the screen. Typically, the user is not allowed to continue or navigate away from a screen when there are data entry errors on the screen. These errors will always be identified by yellow or red highlighting and often accompanied with a more specific error message.

2.3.3 Entering Probability Vectors

There are a number of places in the interface where probability vectors must be entered. These are used to enter probabilities associated with a set of mutually exclusive outcomes. Each uses a

similar graphical interface as can be seen on the Specify Application Times screen (Figure 2.4). This screen contains two probability vectors where the user enters information on how long after a treatment the simulated individual stays out of the treated area. Each probability vector is composed of:

- A container box with a descriptive title. In this case this title is 'Probabilities for Time of Application for Outdoor (Lawn or Garden) Scenarios';
- A series of labeled text entry boxes. In this case 12 of them. Each is labeled and contains a probability;
- A space below the text entry boxes where error messages may be displayed; and
- An OK button used to validate the entry.

Each text box must contain a probability, thus a number between 0 and 1 inclusive. The total of all probabilities must sum to one. The user can enter values in all but the last box (the one with a bold outline). The last box automatically displays the amount necessary to sum all probabilities in the vector to 1. When an inappropriate value is entered by the user, the background will turn yellow and an error message will be displayed. The probability vector as a whole will be validated, and the sum recalculated every time the user uses the return key or when the OK button is clicked. Examples of possible error messages are shown in **Table 2-1**. The error messages are not displayed in some contexts. The text boxes are always highlighted in yellow. If there are errors with individual probabilities or with the sum of probabilities, the user will not be allowed to continue to the next screen. The errors must be corrected and the vector validated, or the Cancel button must be used. No values will be saved if the Cancel button is used.

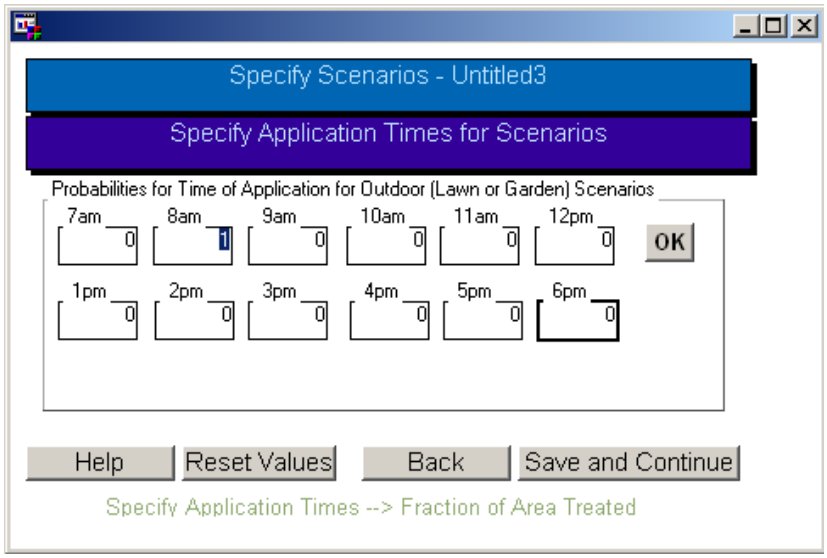
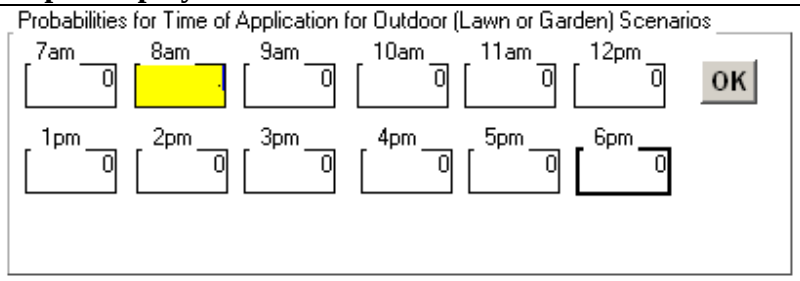
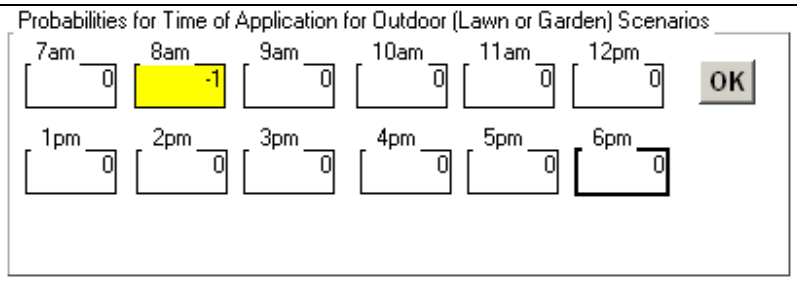
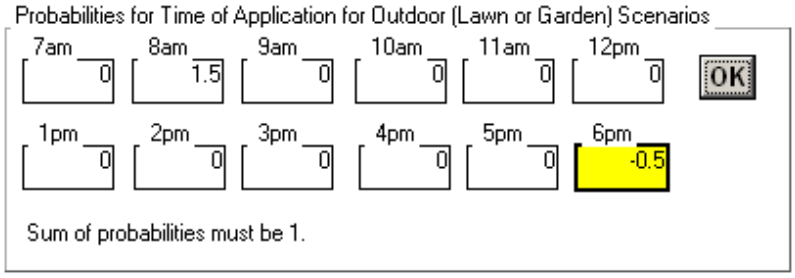
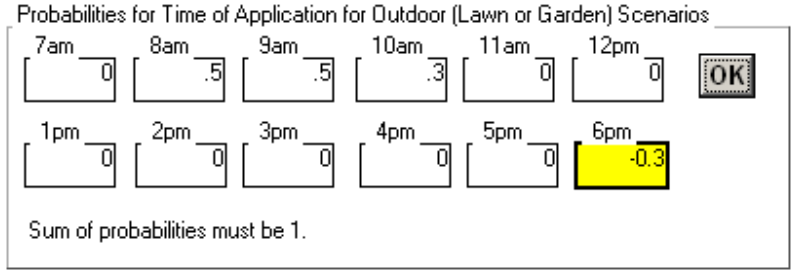


Figure 2.4. Specify Application Times Screen Containing a Probability Vector.

Table 2-1. Probability Vector Errors Encountered

Error	Sample Display
The value entered was not a number.	
A negative value was entered.	
A value outside the range of 0 to 1 was entered.	
The sum of all values entered is too large.	

2.3.4 Distributions Supported

Since the SHEDS-Residential model is a stochastic model, a large number of its input variables are defined by distributions rather than constants. The model supports point values (constants) and 8 distributions. The distributions, parameter names, and rules for the parameters are given in Table 2-2. Detailed information on the distributions and their parameters can be found in the SHEDS-Residential Technical Manual.

Table 2-2. Supported Variable Distributions

Distribution	Number of Parameters	Parameter Names	Rules for Valid Distribution
Point	1	Value	
Uniform	2	Minimum, Maximum	minimum < maximum
Normal	2	Mean, Standard Deviation	standard deviation > 0
Log Normal	2	Geometric Mean (GM), Geometric Standard Deviation(GSD)	GM>0, GSD>1
Triangle	3	Minimum, Mode, Maximum	minimum ≤ mode ≤ maximum, minimum < maximum
Exponential	2	Minimum, Mean	minimum < mean
Gamma	2	Shape, Scale	shape>0, scale>0
Binomial	1	Probability of positive (yes) outcome	0 ≤ Probability ≤ 1
Beta	2	Shape1, Shape2	shape1>0, shape2>0
Weibull	2	Shape, Scale	shape>0, scale>0
Empirical	1	Full filename that containing list of measurements	Plain text file that contains one numerical value on each line.
Uncertainty (Only available for uncertainty runs)	1	Name of SAS dataset containing N uncertainty distributions, one on each observation. Dataset must be saved in the UNC directory under the runname.	Distributions may be of any type; multiple distributions types are allowed within a single uncertainty file. Each distribution definition must follow the rules contained in this table for different types.

2.3.5 Entering Distributions

2.3.5.1 Individual Distribution Widgets

Distribution widgets are an interface object used to enter parametric distributions. They may be found on various interface screens (e.g., Figure 5.27, Figure 5.30, and Figure 5.28) and on the

Edit Variables screen which also includes visualizations of the resulting distributions. The distribution widget (Figure 2.5) is composed of:

- a container box with a descriptive title;
- a pull-down combo box with a list of distributions;
- a series of labeled text entry boxes. The number of text entry boxes varies with the number of parameters required; and
- an OK button to force validation.

Enter a distribution by clicking on the pull-down arrow and making a selection from the list that is displayed. Then enter values for each parameter. Pressing the tab key will move from parameter to parameter. However, you will need to either press the enter key or click the OK button to force the values to be validated. If one or more of the values are incorrect when validated, the background of the container box will turn yellow and you will not be permitted to go to the next screen. Truncation minimum or maximums[1] may be left undefined. The text box containing these values will indicate an error, but the distribution as a whole will still validate.

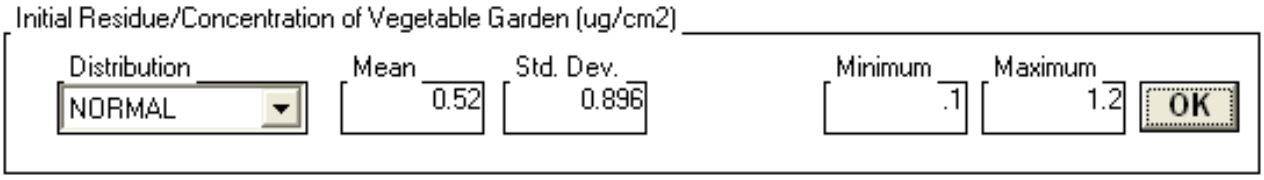


Figure 2.5. Example Distribution Widget.

After entering corrections hit return or click on the OK button to force validation and clear errors. In some contexts specific error messages will be displayed.

2.3.5.2 Entering Empirical Distributions

The "Empirical" distributions type is new for Version 4. This feature allows the users to define an empirical distribution via a list of measurements, rather than using a continuous probability distribution. Empirical distributions are contained in plain text files, with each line of the file containing a single numerical measurement or value. The user creates these files outside SHEDS, and then selects the "Empirical" distribution type in the distribution widget. The interface will then prompt the user for the full path and filename of the empirical data file. The distribution widget will show an error if the file does not exist. An example of an empirical data file and its file specification in the distribution widget for the variable fraction of skin unclothed are shown in Figure 2.6. When this type of distribution is used, each of the values in the file will be sampled with equal probability. The user can enter histogram-type data by using multiple copies of the measurements in the file. For example, the file shown in Figure 2.6 essentially represents a histogram in which 75% of the outcomes are 0.3, 12.5% are 0.2, and 12.5% are 0.4.

1 Distributional parameters do not reflect the effects of truncation.

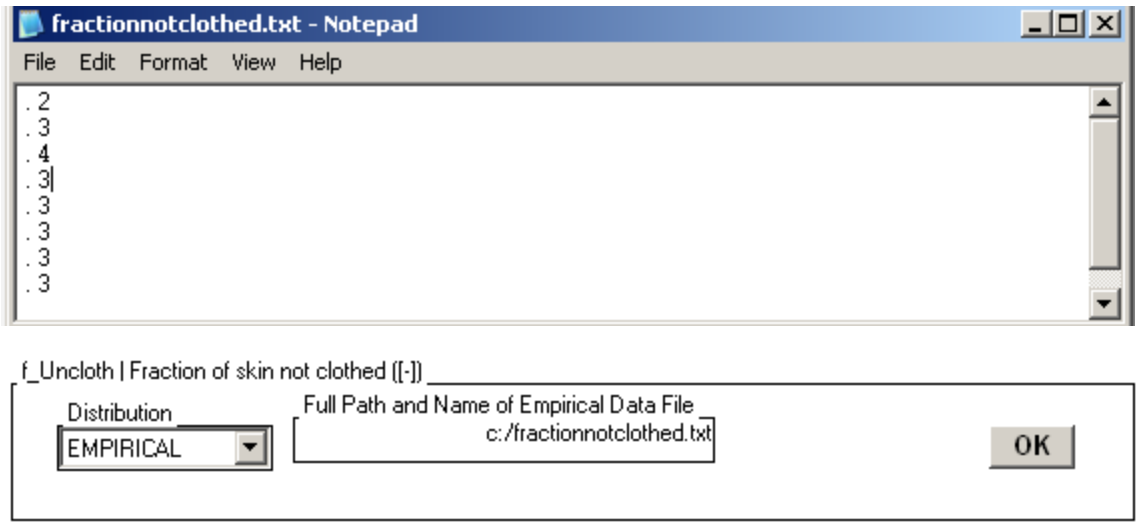


Figure 2.6. Example Empirical Data File and File Specification in the Distribution Widget.

2.3.5.3 Entering Uncertainty Distributions

The "Uncertainty" type of distribution is also new in the SHEDS version 4 GUI. This distribution type is only valid for uncertainty runs and will not be visible for other types of runs. This feature allows the user to define a set, or "cloud" of distributions for a variable, one of which is then selected for use (with equal probability) for each uncertainty repetition. See the SHEDS Technical Manual for more information about uncertainty runs.

The uncertainty distributions must be contained within a SAS dataset, one distribution definition per row. Thus, it is helpful for the user who utilizes this feature to have some knowledge of how to create and edit SAS datasets. Each of the distribution definitions (each row) must contain a valid distribution form (Point, Uniform, Normal, Log Normal, Triangle, Exponential, Gamma, Binomial, Beta, Weibull, Empirical), and the required parameters as defined in Table 2-2. The parameters are given the names V1-V3. Thus for a beta distribution, v1 and v2 (shape1 and shape2) must be defined. Optionally, each distribution may contain a maximum and minimum ("maxval" and "minval") values. For "Empirical" distributions, the filename of the empirical data file is contained in the "empfile" variable.

The user creates the uncertainty dataset outside SHEDS, and then selects the "Uncertainty" distribution type in the distribution widget. The user then must copy the dataset into the folder <SHEDS-Root>\runs\XXXX\input\unc, where XXXX is the run name. Thus the run must already be defined. The interface will prompt the user for dataset name. The distribution widget will show an error if the dataset does not exist in the UNC directory. An example of a valid

uncertainty distribution dataset and its dataset specification in the distribution widget are shown in Figure 2.7. These data are strictly for demonstrations and are not meant to represent the value of any real variable.

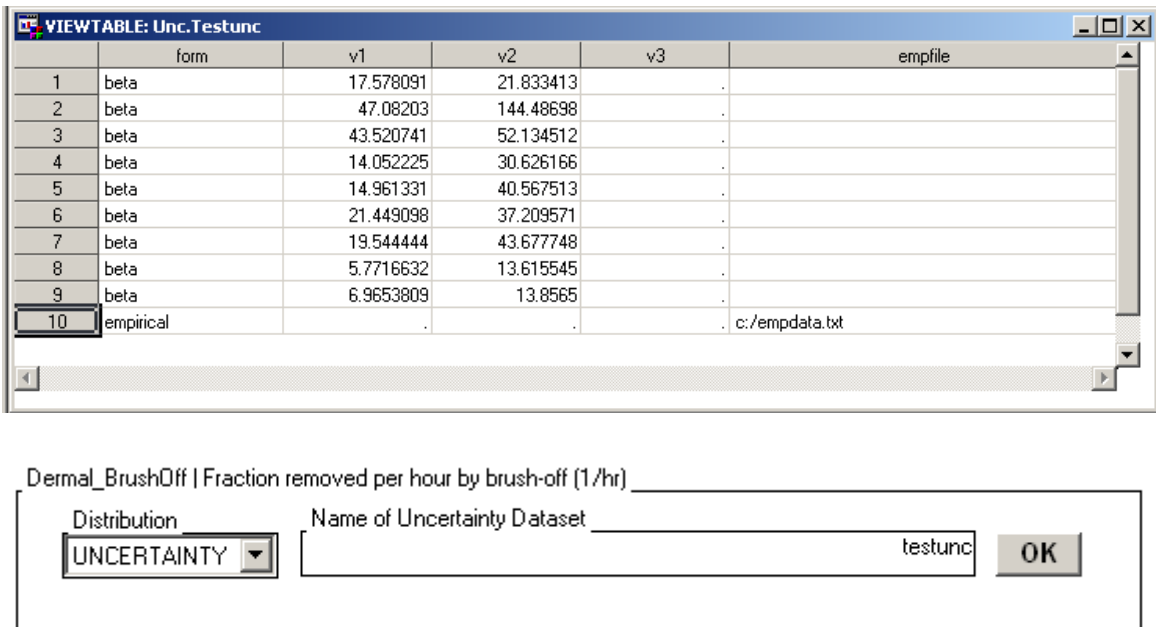


Figure 2.7. Example Uncertainty Dataset and File Specification in the Distribution Widget.

3 Installation

3.1 Requirements

SHEDS-Residential 4 was developed under SAS version 9.1 on machines running MS Windows 2003 and XP Professional.

To install and use SHEDS-Dietary, you will need a computer running 32-bit SAS version 9.1 or higher. A version of SHEDS for 64-bit SAS is available upon request. SAS must be installed prior to installing SHEDS. Your computer hardware needs to be adequate to run SAS and MS Windows. Additionally you should have:

a 600 MHz processor,
64 MB of RAM, and
150 MB of free disk space.

However, it is recommended that you have:

a faster processor,
128 MB or more RAM, and
more than 250 MB of free disk space.

The software should run on other systems where SAS is implemented, but this has not been tested.

Each run will consume about 16MB + (0.28*N) MB where N is the number of people simulated for 1 year. So a run of 200 people will take up 72 MB of disk space.

WARNING: It is highly recommended that the user pause or disable any automated anti-virus or back-up programs that access the SHEDS installation or data output directories, or place these directories in locations that are not virus-checked or backed up. Such programs may access SHEDS data files and interfere with model performance, causing unpredictable results.

3.2 Installation under MS Windows

Installation has been designed so that administrative privileges are not required.

WARNING: If you wish to save the results from model runs, copy the affected results files from the installation directories to another location before uninstalling or reinstalling SHEDS.

3.2.1 Starting With a CD

If you have a CD, do the following:

1. Insert the CD into your CD reader.
2. Use Windows Explorer to navigate to the top level files on the CD.

Double click on the SHEDS_Multimedia_Setup.exe file to initiate the installation. The installation may have version numbers after the "Setup". For instance …Setup_4.14.exe.

3.2.2 Starting with a Downloaded File

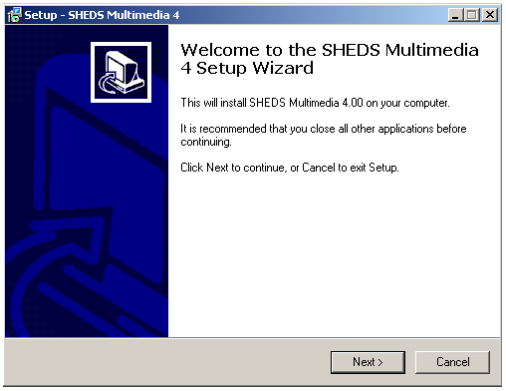
You may obtain the setup file via FTP or another electronic means.

1. Save the attachment to a local or network hard drive. The method you use to do this will vary depending on the program you use to obtain the file.
2. Use the Windows explorer to navigate to the saved file.
3. Double click on the saved file to start the installation.

3.2.3 The Standard Installation Process

Once the installation wizard is initiated, simply follow the instructions. This will install the necessary program and data files, create a program group on the Start menu, and create an icon on the desktop. The desktop icon will execute the interface within SAS. The program group will contain an additional shortcut (menu item) to uninstall the model and program data.

The screens encountered during install, and an explanation of each, are shown in the following figures. For a default install, users should simply continue to click the Next buttons until the final screen.



The initial screen informs the user what version will be installed. Click the Next button to continue

Figure 3.1. Setup Screens: Initial Screen.

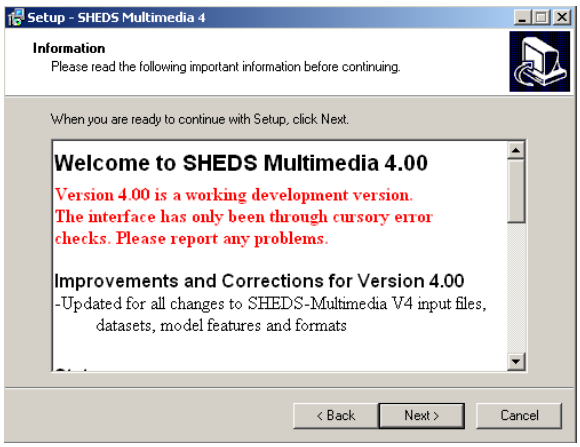


Figure 3.2. Setup Screens: Welcome and Information Screen.

This screen provides some information about the current state of the program and how to get support.

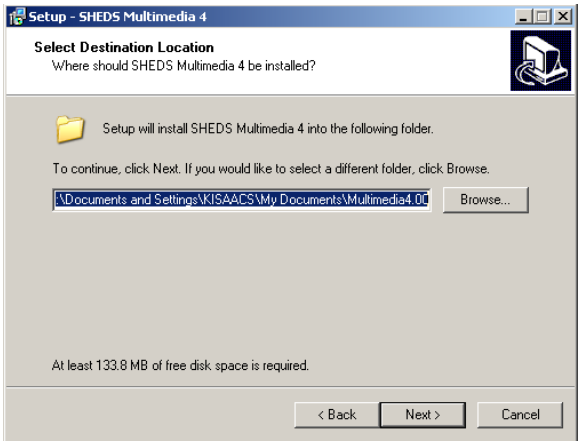


Figure 3.3. Setup Screens: Installation. Directory Screen.

The user may elect to install the files somewhere besides the default location. The default location is in the user's My Documents directory. If the user desires, the Browse button can be clicked and a dialog allowing the choice of an alternate location will come up. The main reason one might want to install somewhere else is that the user generated simulation results are large and by default are stored under the install directory. Note that the user may redirect the output to another location.

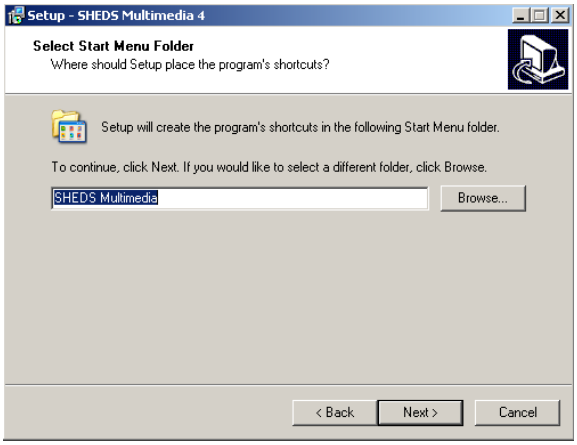


Figure 3.4. Setup Screens: Shortcut Folder Name.

Figure 3.4 shows the final window before install begins. Allows the user to set the name of the program group in the Start Menu. The user should not need to change this.

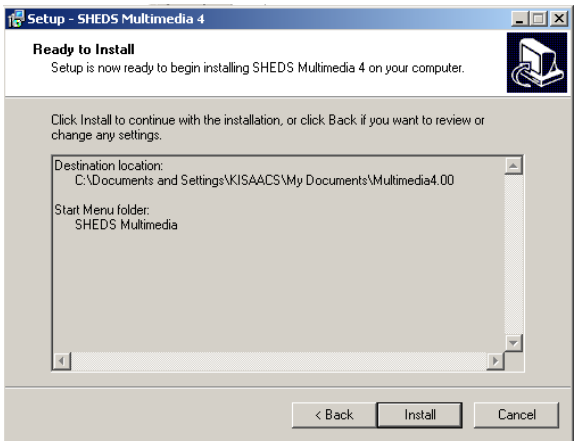
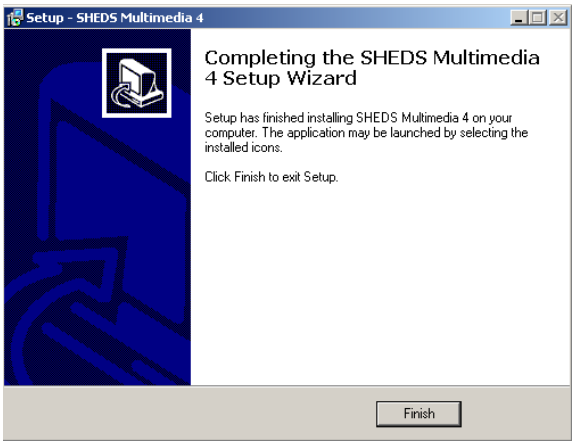


Figure 3.5. Setup Screens: Confirmation Screen.

The user has the chance to review installation specifications on this screen before the installation begins.



After the files have been extracted and placed in the specified install directory, and the desktop icon has been placed, the final screen will indicate that the installation is complete.

Figure 3.6. Setup Screens: Completion Confirmation.

3.2.4 Starting the Model Interface

The installation will place an icon on your desktop. The icon should appear as the standard SAS icon, with the label "SHEDS Multimedia 4". However, this varies depending on the version of SAS the user is running. It will typically include an inverted triangle as part of the icon. Double click on the icon (figure at right) to start SAS and the main screen of the SHEDS Interface.

Figure 3.7. SHEDS Multimedia Desktop Icon.

3.2.5 Removing SHEDS-Residential

If SHEDS was installed using the installation wizard, the user can uninstall it in a manner similar to other Windows programs. **Removal of the program will remove all of the user's simulation output files unless these were saved elsewhere.** To start the removal process, click on the "Uninstall SHEDS Multimedia" choice in the SHEDS Multimedia group of the Programs menu.

4 The SAS User Interface

Most of the SAS user interface provides detailed fine-tuning capabilities that are usually not necessary for typical model use. The average user may still find a brief review of this section useful. If the user is unfamiliar with SAS and wishes to explore raw datasets used by the model, then it is recommended the user read this section more carefully.

4.1 The SAS Screen

Assuming one uses the link in the MS Windows Programs menu or the screen icon to start the model, the main GUI screen will start inside the main SAS window (Figure 4.1). By default, the SAS log window will not open when the program starts, but can be opened by selecting View-> Log on the SAS toolbar.

The SAS window is split into a number of distinct areas. The main area for viewing documents, forms, data sets, and graphs is in the middle. This area may have multiple windows active at one time. The user may activate a particular window by clicking on the title of the window. The bar immediately below this area contains one button for each window in the main area. The buttons indicate which window is active, and allow one to activate a different window. In Figure 4.1, the main SHEDS screen is active as can be seen by the colored title bar and the depressed appearing button. Note that since the main SHEDS screen does not have a title on the title bar, its button is unlabeled. As the SHEDS GUI and model are run, informational and error messages will be displayed in the log window. The pull-down menus are on the top of the screen, just under the title. The toolbar is below this. At the very bottom of the SAS window is a status bar, which will contain help text for many interface features as the user moves the mouse over the GUI.

Additional SAS windows can be opened using the SAS View menu (Figure 4.2). The Graph window displays all graphical output generated. The interface uses a separate output window for this purpose so the Graph window will generally not be needed. It should also be noted, that since the model interface overwrites images of the same type, SAS's graph window may appear unreliable.

The SAS output window is where any tabular output generated is written by default. Generally, the model does not provide this type of output.

The Results window (Figure 4.3) provides a list of tabular and graphical results generated and printed to the graph and output windows. It is generally locked on the left side of the SAS window. If additional windows are locked in this area, they are accessed with tabs that appear below. The Results window may be used to navigate among the different outputs. However, it will not open the output or graph windows; this must be done manually.

The Explorer window (Figure 4.4) is used to navigate through SAS libraries and files, data sets, forms, and programs. It can be used to access the raw files used as input or output to the model.

This screen may float in SAS's main area or it may be locked on the left side of the SAS window and be accessed via a tab on the bottom of this area. This screen may be toggled between tree mode (shown) and a single pane, similar to MS Windows Explorer.

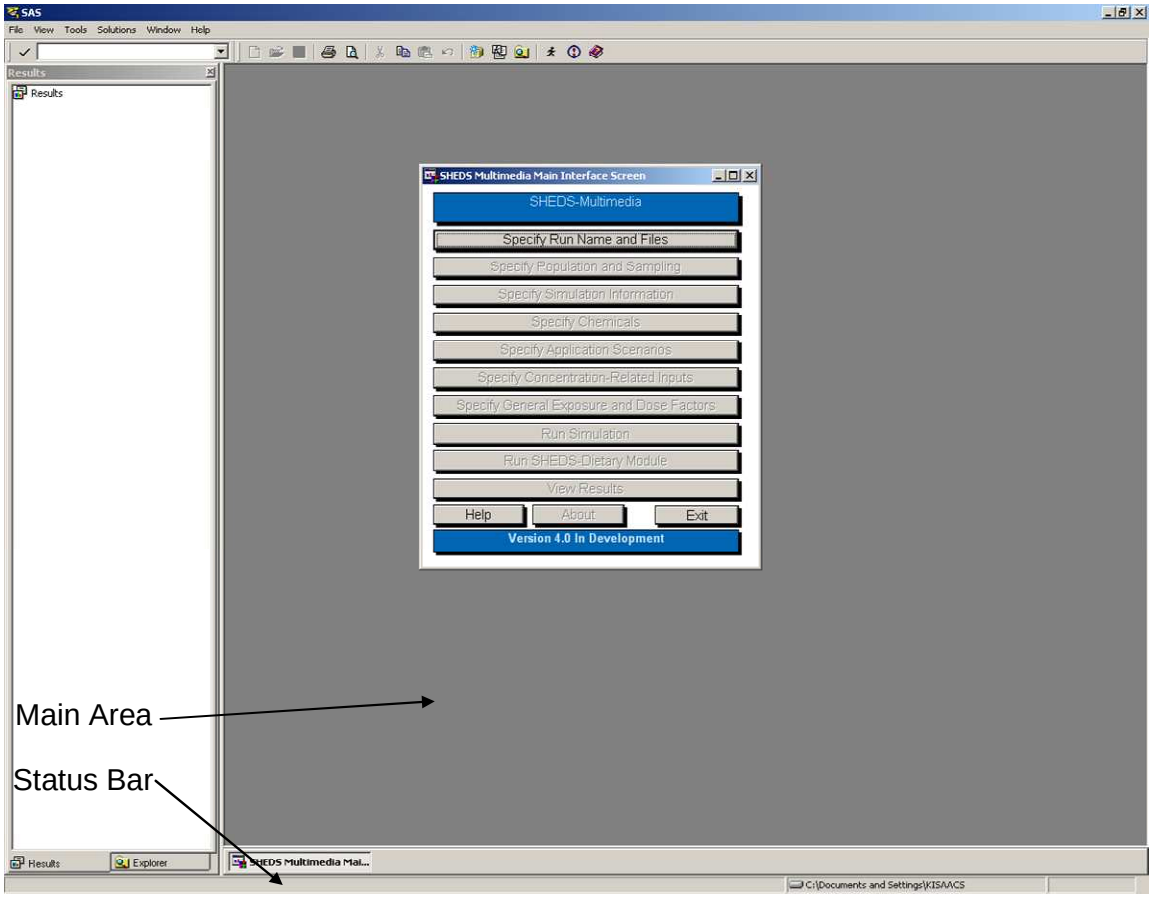


Figure 4.1. The Main Model GUI Interface Screen in the SAS Window on Startup.

Figure 4.2. The SAS Menu Bar and the View Menu.

Figure 4.3. The SAS Results Window.

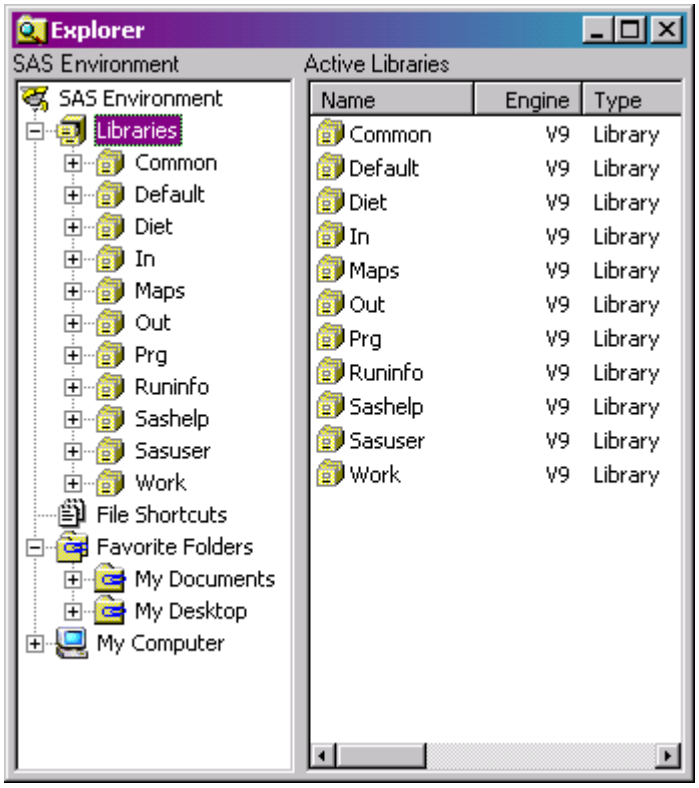


Figure 4.4. The SAS Explorer Window.

5 SHEDS-Residential: The Graphical User Interface

5.1 SHEDS Mode

When SHEDS-Residential is started, the first screen the user will encounter is a Disclaimer screen that provides some general information about SHEDS and indicates how to receive support. After this screen, the user will encounter an initialization screen that asks the user whether they want to run SHEDS in Aggregate or Cumulative Mode (Figure 5.1). If only single-chemical runs are going to be performed, the user may want to use Aggregate Mode, as some screens will be bypassed in this mode. However, single chemical runs can also be created in Cumulative mode, but the user may have to pass through a number of screens that are bypassed in Aggregate mode. Multi-chemical runs can only be created in Cumulative mode, and any defined multi-chemical runs should not be examined in Aggregate mode, as the behavior or the interface will be unpredictable. However, single chemical runs that are created in Aggregate mode can later be viewed and edited in Cumulative mode, for example, should the user want to add chemicals to an existing run.

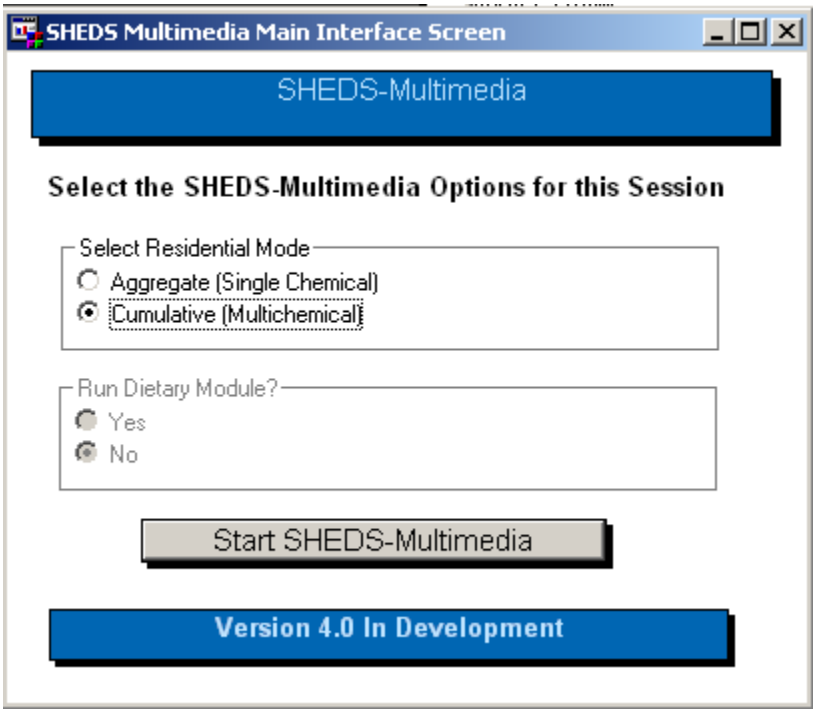


Figure 5.1. The SHEDS Mode Screen

5.2 SHEDS-Residential Main Interface Screen

After the SHEDS-Mode screen is completed, the main screen will be displayed (Figure 5.2). This is the main interface window that you will be returned to after completing each main step. It contains the following buttons.

Specify Run Name and Files: Choose or define a new run name, identify existing input files.

Specify Population and Sampling: Define basic information for the run: number of people sampled, type of run (variability, sensitivity, or uncertainty), ages of interest. Subset the CHAD database.

Specify Simulation Information: Define the length of simulations, source-to-concentration approach, and a number of other global simulation variables.

Specify Chemicals: Specify the chemicals to be included in the run and their general properties.

Specify Application Scenarios: Specify the application scenarios to be used in the run. Define the dates and times of applications, reentry times, and relationships between application dates.

Specify Concentration-Related Inputs: Specify decay and dispersion inputs, or interval distributions, or time-series data.

Specify General Exposure and Dose Factors: Specify all other inputs including transfer variables, input variable correlations, etc.

Run Simulation: Run the current simulation.

Run SHEDS-Dietary Module. This is a non-functional placeholder button. In the future, this interface may be linked with the SHEDS-Dietary model.

View Results: View results from previous runs.

Help: Bring up the contents for the help screens.

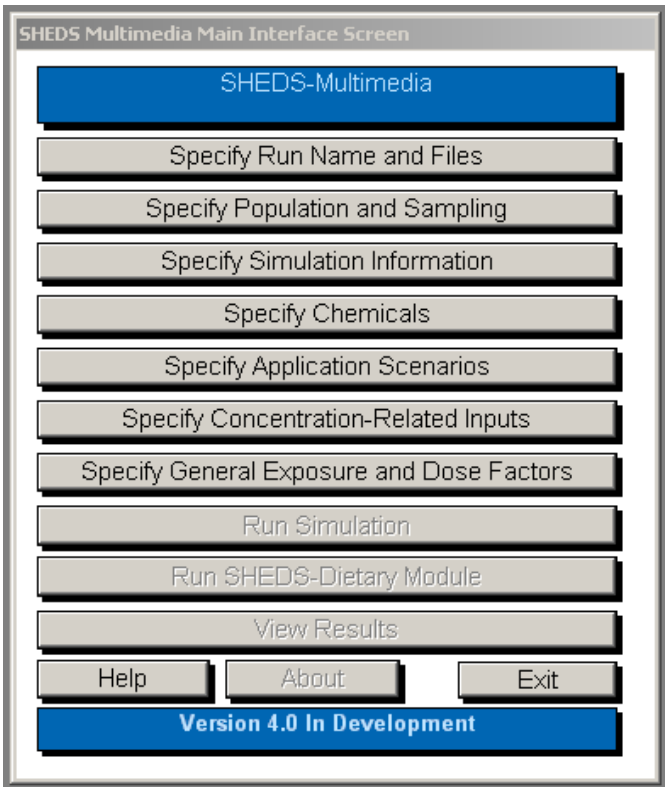


Figure 5.2. SHEDS-Residential Main Screen.

About: Bring up the help screen describing this version of the model (to be implemented).

Exit: Close the SHEDS user interface.

These buttons allow the user to move through the proper sequence of steps to conduct a new model run, or to view results and manage files from previous SHEDS simulations. Initially only one button will be enabled (Specify Run Name and Files). Buttons that are not enabled are displayed with a gray tint to the font. The initially enabled buttons are Specify Run Name and Files and Exit.

Before beginning to specify the inputs for a new simulation run, editing the inputs for an existing simulation, or viewing the results of a previous run, the user will need to specify the run name. The run name is simply a title for a simulation run that references all input files for and output files from a run.

Clicking on the "Specify Run Name and Files" button will bring up a screen allowing the user to enter the run name. After specifying the run name and if necessary, the files (see below), the user will be returned to the Main Window. If setting up a new run the Specify Population and Sampling button will now be enabled. If viewing the results of a previous run, then the View Results button will be enabled. The appropriate buttons will be enabled as the user completes each step, and returns to the main menu.

5.3 Specify Run Name and Files

The first step in SHEDS-Residential version 4 is to click on the "Specify Run Name and Files" button. The run name is like a file folder that keeps together all the information specific to a simulation. In technical terms, it relates to a directory where files are stored and a record in a database that stores information about a run.

5.3.1 Specify Run Name Dialog

The Specify Run Name dialog (Figure 5.3) allows the user to do several things:

Edit Selected Run: Restore the contents of a previous run for editing. When this simulation is run, any results from previous submissions of this run will be overwritten.

Copy Selected Run To New Run: Use the same inputs from a previous run in a new run and allow them to be edited. This avoids erasing the output from the previous run.

Create a New Run: Enter a new run name and begin defining inputs.

View Results of Selected Run: Select run so that the user can view its results. Edits of the inputs are not allowed and the run cannot be re-submitted.

Delete Selected Run: Delete an existing run.

The "Specify Run Name" dialog is composed of three main parts: The first is a list box containing the names of previously defined simulation runs. The currently selected run name is highlighted in this box. Below the list box, the description of the currently selected run name is displayed. This provides additional information on the run. The user enters it when the run is created. On the right of the dialog are the action buttons. These perform an action, usually on the selected run name. As in other dialogs the "Help" button (when implemented) will bring up a help screen for this dialog. The Cancel button closes the screen without selecting a run name.

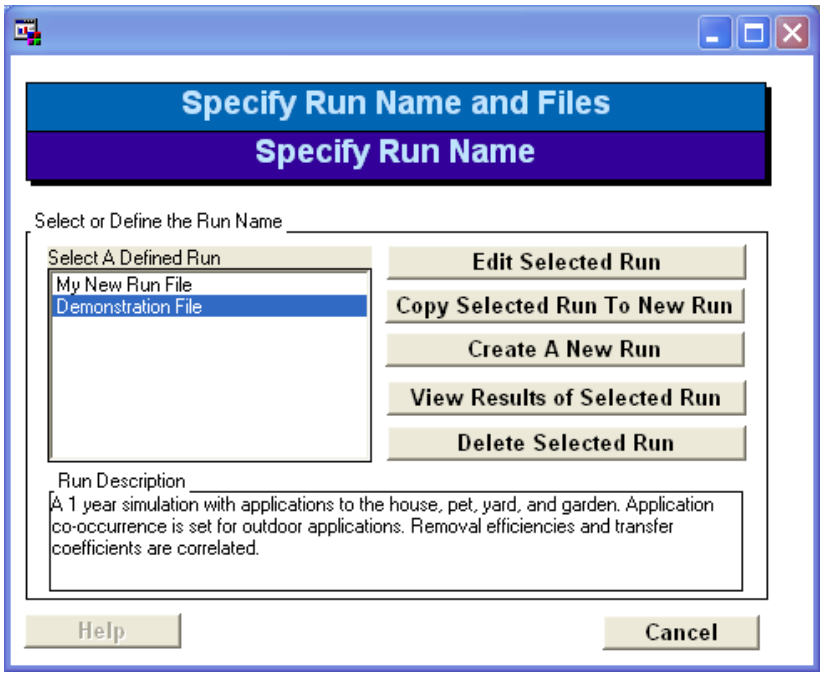


Figure 5.3. Specify Run Name Screen.

To select an existing run name simply click on that name in the "Select A Defined Run" list box. In most cases the user will need to select a run name before clicking on the action button.

5.3.1.1 Edit Selected Run

This button allows the user to continue editing an existing run. The user will be taken to the "Specify Files" screen (Figure 5.5). After that the user will be returned to the main menu. This feature is useful, for example, if one is interrupted in the process of creating a run. The inputs already entered may be saved and SHEDS exited. To finish creating the run, one selects the incompletely specified run, chooses this "Edit" button, and continues defining the run. This button is also useful in changing inputs on a previously completed run, if the user is willing to overwrite the previous inputs and the resulting output. When becoming familiar with the model using the Demonstration Permethrin Case Study it is recommended that you use the Copy Selected Run to New Run since any changes made using the Edit Selected Run button would overwrite the original file.

5.3.1.2 Copy Selected Run To New Run

A run name should be selected before clicking on this button. The information for that run will be copied. The user will be allowed to define a new run name using the "Enter New Run Name" screen (Figure 5.4) and will then be taken to the Specify Files Dialog and allowed to edit information there. As distinct from the "Edit Selected Run" button, this button is used to modify

inputs from a previous run, save the changes into a new run name, and still maintain the inputs and outputs from the original run.

5.3.1.3 Create a New Run

To create a new simulation from scratch, click on "Create A New Run". The "Enter New Run Name" screen (Figure 5.4) will appear allowing the user to enter the new run name and description. After this is completed, the "Specify Files" screen will be displayed (Figure 5.5). Initially, defaults for all values will be used. Note that the chemical-specific default input values provided for the case study in SHEDS-Residential version 4 are for Permethrin, and the user must change them to fit their own chemical or scenario data. Chemical-specific inputs not used in the case study are set to a point value of zero.

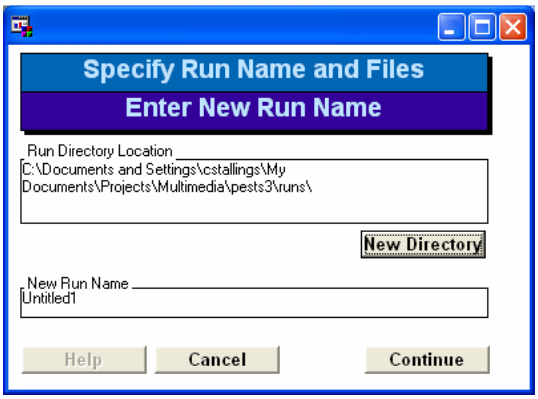


Figure 5.4. Enter New Run Name screen.

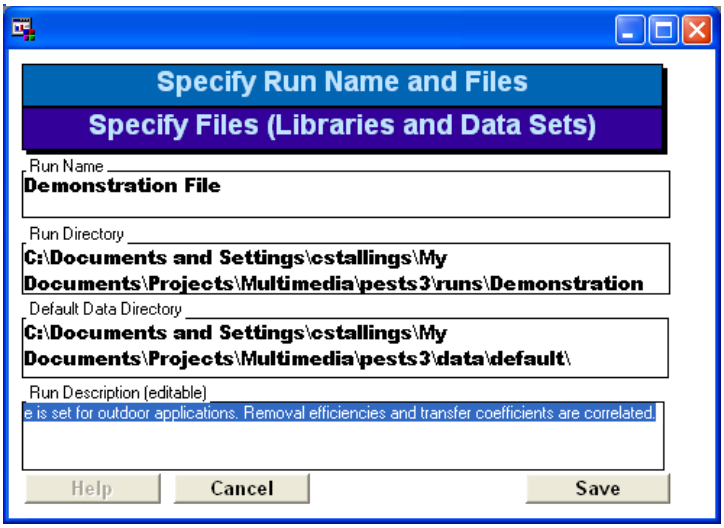


Figure 5.5. Specify Files Screen.

5.3.1.4 View Results of Selected Run

Clicking this button chooses the currently selected run name and returns the user to the main menu where the "View Results" button will be enabled. This will allow the user to view output from the selected run. The user will not be allowed to view or edit run inputs in this model.

5.3.1.5 Delete Selected Run

Clicking this button deletes the selected run name from the database. After a dialog confirming that the user wants to delete the run information (Figure 5.6) the user is returned to this dialog.

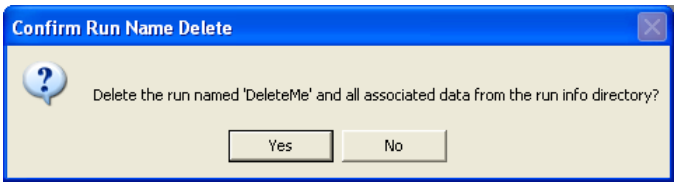


Figure 5.6. Confirm Delete dialog.

5.3.2 New Run Name Dialog

The dialog shown in Figure 5.4 allows the user to enter a new run name and a directory path in which to store the results. This screen is accessed when the user clicks on either “Create A New Run” or “Copy Selected Run To New Run” from the Run Name Dialog. There are three cases for the directory path. When copying from another run, this box shows the location of the prior run and the user can change this. When creating a new run, this box displays the storage location of the last run. If there is no prior run (immediately after the installation), this box displays the default run location.

The default run name is “UntitledN” where N is the next integer after the last stored untitled run. The user may enter any valid Windows file names. After entering the run name, press return and then click on the Continue button. If the name is the same as a previously used name an error will be displayed and the user will be allowed to enter a new name. Clicking on continue will in general take the user to the “Specify Files” Screen

5.3.3 Specify Files Dialog

When creating, copying, or editing a run, the user will reach this dialog (Figure 5.5). This dialog allows the user to verify the main directories and specify alternate dietary inputs.

The very top of the dialog simply displays the current run name and run directory. The run directory should be similar to the run name, but altered so that it is a valid directory name. The input and output files from the simulation run will be stored in this directory. The default data directory is where the basic model input data is stored.

The run description will be displayed and may be edited in the next box down.

The “Cancel” button will leave the dialog without saving any changes. The user will return to the Specify Run Name Dialog. The “Save” button will save any changes, and return the user to the main menu.

When the Specify Files dialog is initialized, the SAS libraries are also set up for the simulation run or simulation results. If setup was for some reason not carried out correctly upon installation, various errors may occur at this point. In this case, reinstallation is recommended.

5.4 Specify Population and Sampling

Clicking on this button of the Main Window displays the related screen (Figure 5.7). The run type is selected via the Sampling Method selection box. Five different types of runs are available through the interface: variability runs, uncertainty runs, and three types of sensitivity analysis runs: percentile scaling, Sobol's method, and input-output correlation. In practice, the uncertainty and sensitivity analysis runs make use of multiple repetitions of variability runs; therefore, the variability results are produced for all run types. When "Uncertainty and Variability" is selected as the run type, a box appears (Figure 5.8) that allows the user to specify the number of uncertainty repetitions that are going to be performed. When either "Percentile Scaling" or "Sobol's Method" is selected, an additional button (Figure 5.9) appears that takes the user to a new screen where settings specific to the selected method are entered (see next sections). The input/output correlation method requires no additional input; see the Technical Manual for details of this type of sensitivity analysis.

The user may also enter a random number seed for the run. This seed initializes the random number stream used for all random sampling performed by the model. By setting this value to a positive integer, the user can repeat simulation runs. If the seed is set to 0, SAS chooses a random number seed from the system clock. This seed is saved; when the user reopens a run has already been run, the seed value used will be written in the text box. If the user wishes to repeat the run with new simulated persons, they must reset this seed to a different integer or to 0.

In the "Population: Age Groups and Sample Size" box, the user selects gender(s) and age(s) of interest in the simulation (all ages, or some subset of those ages are available for selection). The "Population Size" option allows the user to specify the sample size for the 1-stage simulation. SHEDS contains two different sets of age group definitions ("EPA Age Groups" and "Optional Group Definitions"); the user can decide which to use.

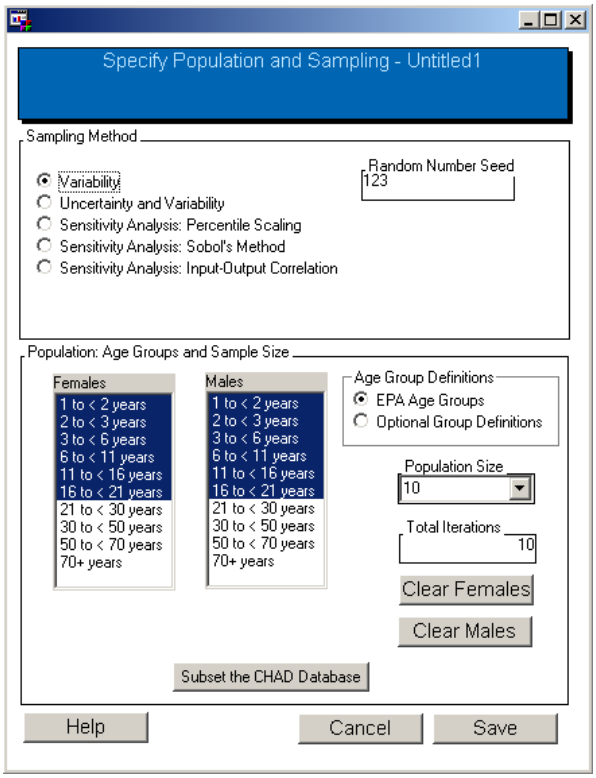


Figure 5.7. Specify Population and Sampling Screen.

Clicking on either “Clear Males” or “Clear Females” allows the user to specify a single gender simulation. Once cleared, cohorts can be added back by clicking on them.

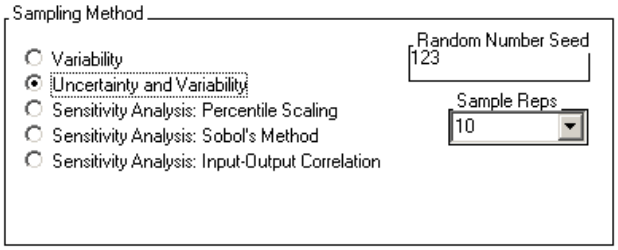


Figure 5.8. The Sampling Method selection box for an uncertainty run.

The time taken to carry out the simulation increases linearly with the Size of Population and Number of Populations selected. There is a lesser increase in run time if longer time-periods are chosen. Depending on the computer hardware, a run of 1000 persons will typically take about an hour to complete.

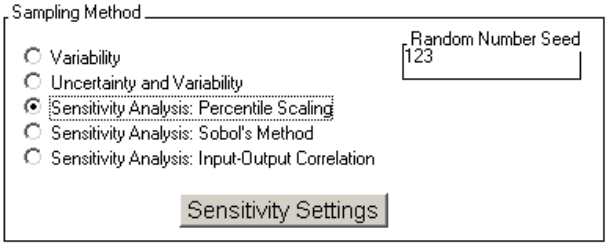


Figure 5.9. The Sampling Method selection box for a Percentile Scaling or Sobol sensitivity run.

SHEDS-Residential makes use of EPA’s Consolidated Human Activity Database (CHAD). CHAD contains human activity diaries from a number of different studies (see the Technical Manual for further information). The user can also choose to select a subset of these studies for use in a run. When the user clicks the “Subset the CHAD Database” button, the screen seen in Figure 5.10 appears. By default, all the studies in CHAD are selected. The user can click on any study to unselect in and remove it from the run. Note that if the user chooses to include a small number of studies, the run may fail due to inadequate numbers of diaries being available for certain age groups, day types etc. If this happens, an error will be written to the SAS log when the run is initiated.

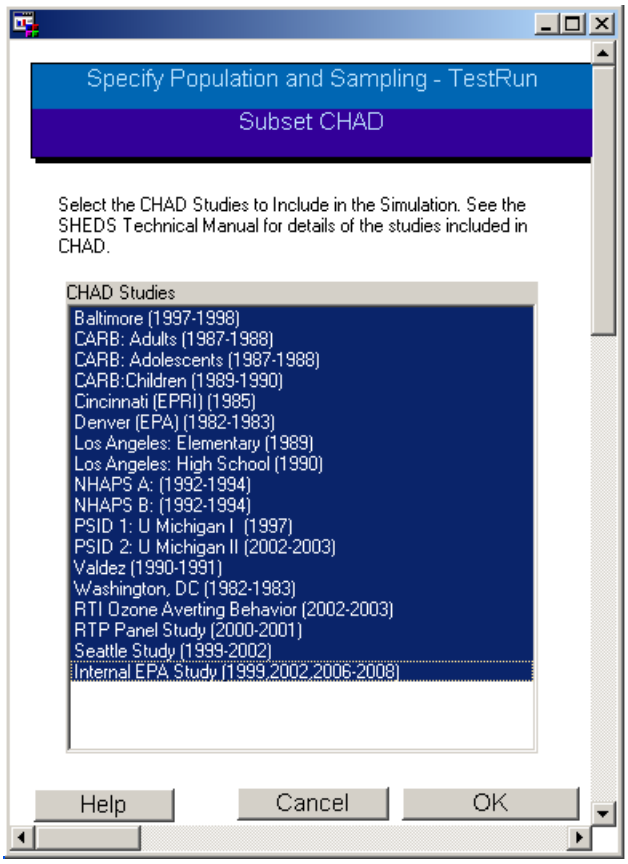


Figure 5.10. Subset CHAD Screen.

5.4.1 Specify Sensitivity Settings

For Percentile Scaling and Sobol's Method sensitivity runs, some additional input is required by the user. This information is entered on one of two screens that appear when the "Sensitivity Settings" button (Figure 5.9) is clicked.

5.4.1.1 Percentile Scaling Run Settings

When performing a Percentile Scaling run, the screen shown in Figure 5.11 appears when "Sensitivity Settings" is clicked. This screen contains a list of all the variables in the run whose sensitivity can be examined. The user selects the variables to analyze by highlighting them in the "Variables Remaining" list and moving them to the "Variables Selected for Sensitivity Analysis" list via the arrow buttons.

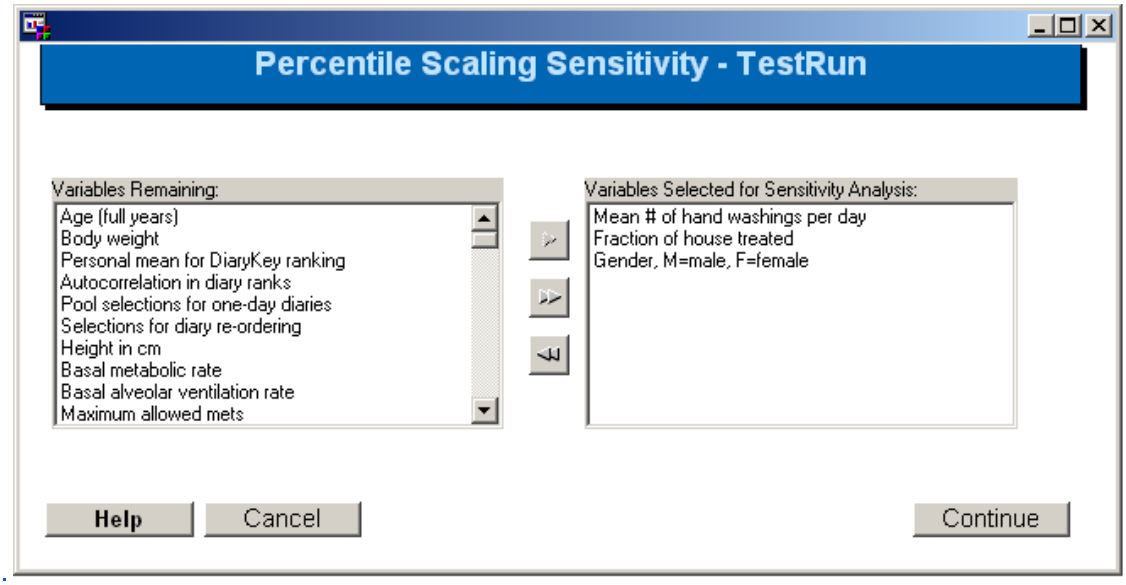


Figure 5.11. Sensitivity Settings: Percentile Scaling Method.

Note that selecting more variables for analysis results in a longer SHEDS run. The total number SHEDS variability repetitions that will be performed in a Percentile Scaling run is 2N+1, where N is the number of variables selected. The percentile method performs a baseline run plus two runs for each variable analyzed: one with the variable set to a high percentile and the other with it set to a low percentile. See the Technical Manual for more information about sensitivity runs.

5.4.1.2 Sobol's Method Run Settings

When performing a Sobol's Method run, the screen shown in Figure 5.12 appears when "Sensitivity Settings" is clicked. This screen contains a list of all the variables in the run whose sensitivity can be examined. The purpose of this screen is then to take these variables and sort them into groups ("Sobol Groups"). The model then assesses the influence of each group on the model output. The user selects the variables to assign to each group by highlighting a group, then highlighting one or more variables in the "Variables Remaining" list and moving them to the "Variables in this Sobol Group" list via the arrow buttons. All of the variables must be assigned to a group; the user will get an error if the "Continue" button is clicked while variables remain. Groups can consist of a single variable if the user wishes to ascertain the influence of that variable alone. However, the number of runs being performed is dependent on the number of Sobol Groups, so caution is needed when defining a large number of groups. The total number SHEDS variability repetitions that will be performed in a Sobol Analysis run is 2N+2, where N is the number of Sobol groups defined. Thus performing runs with a large number of groups may be time-prohibitive. It is recommended that Sobol's analysis be used in a hierarchical fashion. First, an analysis is performed with a few Sobol groups, which perhaps could eliminate a large

number of variables as being non-influential, and identify a subset of important variables. Then further runs could be performed that examine the variables contained in the influential groups more completely. See the SHEDS Technical Manual for more information about Sobol's Analysis.

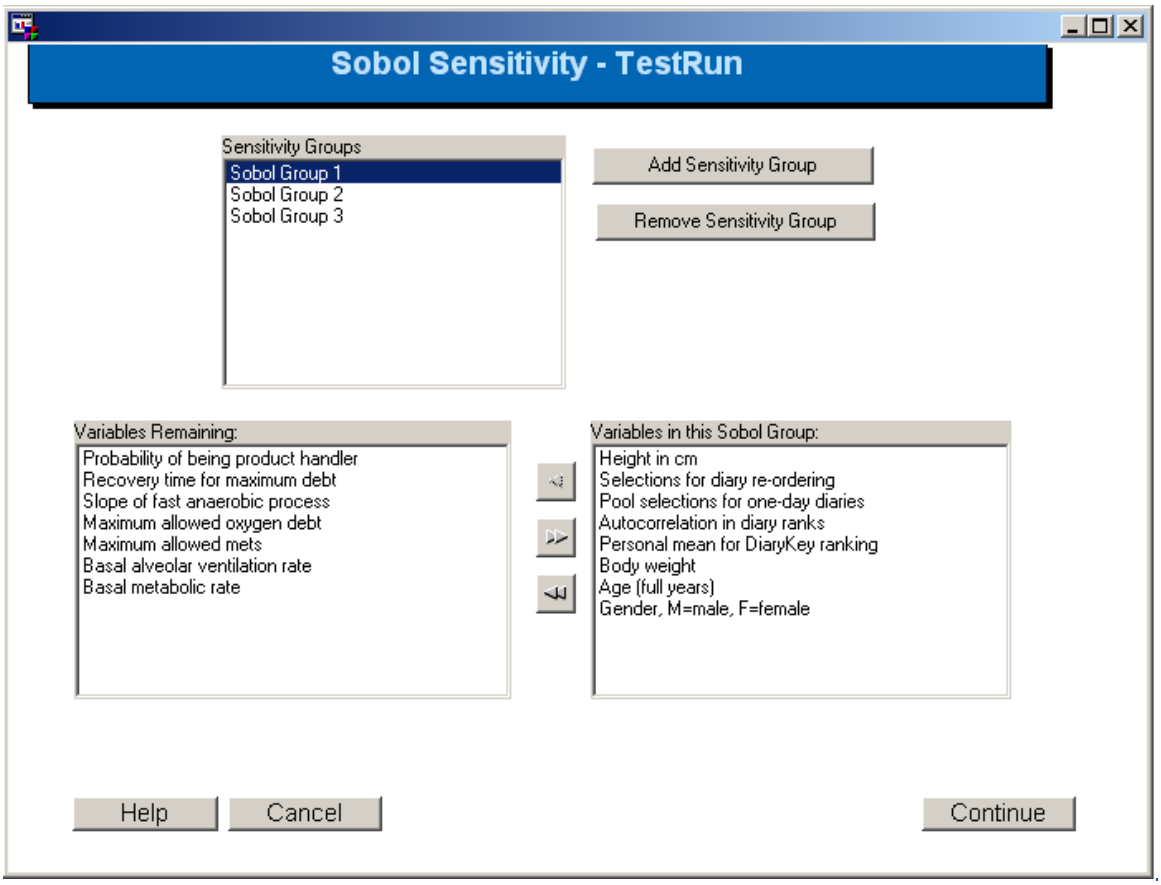


Figure 5.12. Sensitivity Settings: Sobol's Method.

5.5 Specify Simulation Information

This screen (Figure 5.13) allows the user to select a number of options that determine overall simulation variables; each is discussed shortly. Clicking the "Save" button commits any changes. The "Cancel" button prevents changes from being saved.

5.5.1 Simulation Length

The box labeled "SIMULATION START AND LENGTH" allows the user to specify the beginning date (month, day, and year) and the number of days the simulation will track each individual. One common choice of simulation period is to start on January 1st and continue for 1 year (365 or 366 days). However, the model allows a great deal of flexibility. A simulation may begin on any day of the year and can be as short as one day or as long as desired and may cross calendar years. However, caution should be exercised when specifying very long periods as they take longer to run and the model does not alter many personal variable settings (including age) over the simulation period.

5.5.2 Source-To-Concentration Approach and Application Dates

There are three options to generate residues and concentrations for scenario-relevant media:

- **Decay/Dispersion Model:** Specific applications leave a residue on surfaces, in the soil, and in the air. These residues decay with time and are moved to untreated areas.

- **Interval Distributions:** Specific applications leave residues on various media. The concentrations on the media are determined by distributions that change with the time since the application.

- **User-Specified Concentration Time Series:** The user supplies a time series of concentrations for each medium.

The Decay/Dispersion model is a built-in source-to-concentration model that requires the user (in subsequent screens) to enter application and decay rates, and the ratio of residue concentrations in untreated to treated media for indoor applications. Additionally, background distributions can be defined for the various media when Decay/Dispersion is used.

The Interval Distributions selection will require the user (in subsequent screens) to enter distributions of relevant media residues and concentrations for discrete post-application time periods (<1 day, 1-7 days, 8-30 days, 31-365 days).

The User-Specified Concentration Time Series option will require the user (in subsequent screens) to enter time series of residues and concentrations for each medium of interest (e.g., from a measurement study or outputs from an external source-to-concentration model).

If either Decay/Dispersion or Interval Distributions are chosen, a box will appear (to the right of the Source-To-Concentration radio box in Figure 5.13) that allows the user to specify whether the application dates will be User-Specified or Model-Determined. Details will be input on subsequent screens. For user-specified dates, the user will enter specific day numbers for each application type, where day 1 is the first day of the simulation period. Applications will always occur on the dates given. For modeled dates, the user will specify probability vectors for month, day of week, number of applications, and time of applications.

5.5.3 Dermal Exposure Method

For dermal exposure, the user can select the Transfer Coefficient approach or the Transfer Efficiency approach. These two methods are described in the SHEDS-Residential version 4 Technical Manual. Changing this value on a previously defined run will result in the user having to visit the Specify General Exposure and Dose Inputs screen to define related variables.

5.5.4 Diary Assembly Method

SHEDS-Residential version 4 allows the user to select one of two algorithms for constructing the longitudinal human activity diaries for each person upon which the exposure time-series are based. The first method (the Eight Diary method), uses repetitions of 8 activity diaries for each person (a weekday and weekend diary in each season) to construct the year-long diary. The second method selects diaries from the CHAD database based on an algorithm that reproduces certain population statistics, diversity (D) and day-to-day autocorrelation (A), for a key diary variable relevant to exposure for the pollutant being studied. If this option is selected, the user must provide target D and A values for the population, as well the diary variable to be targeted. The available key diary variables are as follows:

- Time Spent Outdoors
- Time Spent Outdoors at Home
- Time Spent Outdoors (Not at home)
- Time Spent in Travel
- Time Spent in Vehicles
- Time Spent in Residences
- Time Spent Indoors (Nonresidential)
- Time Spent at Work
- Time Spent at School
- Time Spent Indoors While Awake
- Time Spent at Home While Awake
- Time Spent Outdoors While Awake

See the SHEDS Technical Manual for more information on the longitudinal diary algorithms and parameters.

5.5.5 Simulate Product Handlers

SHEDS-Residential version 4 allows the user to model persons who specifically handle the chemical of interest in their own home (not professional applicators). If this options is selected, the user will be required to enter additional information later in the interface (see Section 5.8.3), that determines how many of the simulated profiles are handlers and the chemical concentrations that they experience. If handlers are to be modeled, the user must specify a minimum age for handlers; no profiles younger than this minimum age will be identified as chemical handlers.

5.5.6 Export Data For PBPK Model

SHEDS-Residential version 4 allows the user to export SHEDS exposure time series so that the files can be read by an external PBPK model. When enabled, this option produces one extra SAS data set and two text files in the run output directory, in addition to the usual output files.

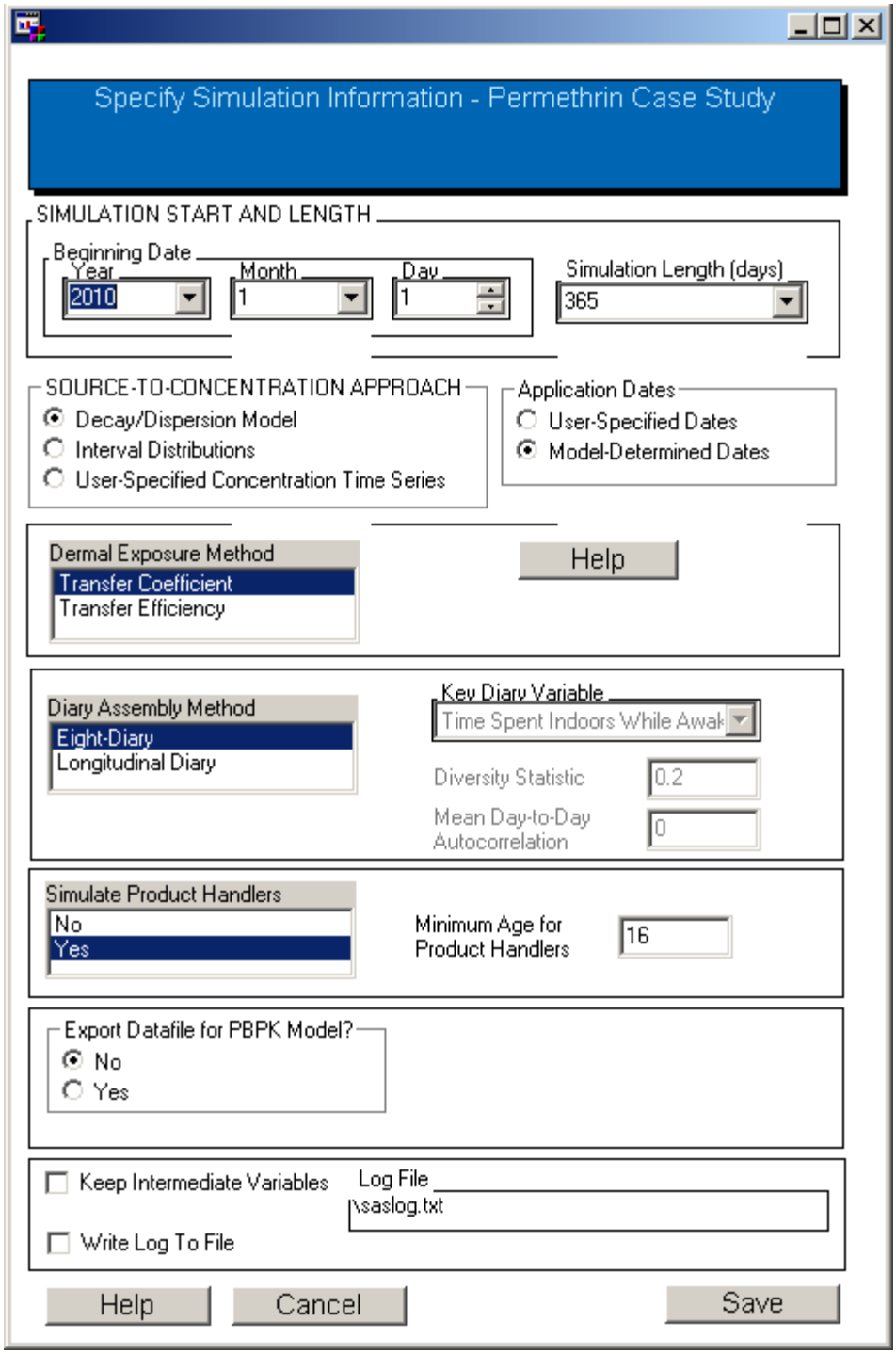
5.5.7 Keep Intermediate Variables

If the user checks the "Keep Intermediate Variables" box, SHEDS will retain variables used in intermediate calculations for simulated individuals. This is useful to check the internal workings of the model.

5.5.8 Save the Log File

To save the log that is generated during the simulation run, the user can click on "Write to Log File" which saves the log to a permanent file outside SAS, thus ensuring the log is saved even if SAS crashes during the run. With this option the standard SAS log screen is not used, so the user cannot track the progress of the run during execution.

If the log file is not saved, a line of output is written to the log window before each individual is simulated, and this is the best way to tell how the simulation is proceeding. If the log is written to a permanent file, the user can open the file with a text editor from time to time to check the status of the run. The name of the log file is fixed. It is stored in the output library.



Note: To utilize the co-occurrence option, the user must select Model-Determined Dates on this screen. The user must also select Specify Parameters before clicking the Specify Inputs button on the Specify Application Scenario Details screen for each scenario for which co-occurrence inputs are to be specified. Application co-occurrence is explained in section 5.7.6.

Figure 5.13. Specify Simulation Information Screen.

5.6 Specify Chemicals

SHEDS-Residential version 4 is a multichemical model. Thus, the user has the opportunity to select or define which chemical(s) of interest are to be modeled in a specific SHEDS Run. This information is specified in the Specify Chemicals screen (Figure 5.14).

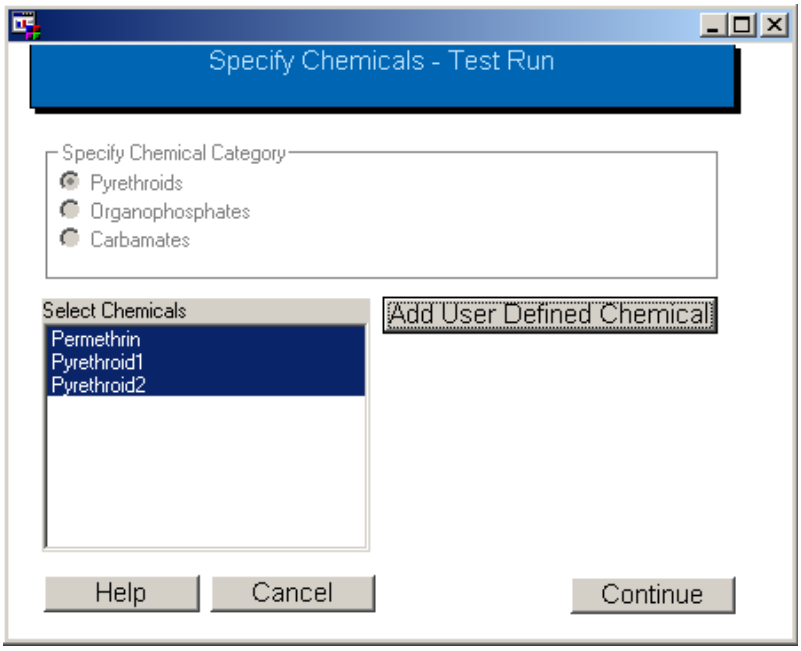


Figure 5.14. Specify Chemicals Screen.

Currently, SHEDS contains default chemical-specific information for Permethrin and two additional pyrethroid chemicals (here, generically called Pyrethroid1 and Pyrethroid2). Note that these chemicals are initialized with the same data as for Permethrin; the user may alter the values as they step through the interface. In the future, SHEDS may contain default data for other chemical classes such as organophosphates, carbamates, or metals.

The user selects the chemicals to include in the run by clicking on the name of the chemical in the Select Chemicals list. Highlighted chemicals are selected for simulation, and the user will be asked to enter information for each of the selected chemicals on future screens.

In Aggregate Mode (see Section 5.1) runs, the user can select just a single chemical at this point. However, it is a valid option for the user to select a single chemical in Multichemical (Cumulative) mode. SHEDS will operate identically as in Aggregate Mode, with the exception that the user will have to visit a few screens that may be bypassed in Aggregate mode (such as assigning chemicals to scenarios; see Section 5.7.3).

5.6.1 Add a User-Defined Chemical

The user may opt to define their own chemical(s) completely from scratch, rather than base their simulation on the defined SHEDS default data for permethrin. In this case, the user clicks the "Add a User-Defined Chemical" button on the Specify Chemicals Screen, upon which an additional widget (Figure 5.15) appears. The user then enters a name for the new chemical, and clicks "OK". The new chemical will be added to the Select Chemicals list, where the user can then select it to be included in the current run. All chemical-specific input data for user-defined chemicals will be initially populated with point distributions having a value of zero, rather than with the default Permethrin data. Thus the user must carefully update any input distributions for their new chemical to reflect their own data.

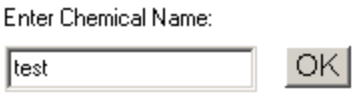


Figure 5.15. Enter Chemical Name for User-Defined Chemical.

5.6.2 Specify Chemical Information

Once the user completes the Specify Chemicals screen, they will proceed to the Specify Chemical Information screen (Figure 5.16). On this screen, the user enters the following information:

- Metabolite name. The name of the bioactive metabolite of the chemical being studied.
- Chemical/Metabolite mass ratio. The ratio of the chemical mass to that of its bioactive metabolite.
- NOAELs. The user must enter the No Adverse Effect Levels (NOAELs) for dermal, ingestion, and inhalation exposures.

The user must complete this information for each of the chemicals in the run. All the chemicals in the run are visible in the Chemicals list box; the user clicks on each chemical in turn and enters the data. The user can not move onto a different chemical if there is an error in the data for the current chemical; in this case the error will be highlighted in yellow and the user must correct it before another chemical can be selected.

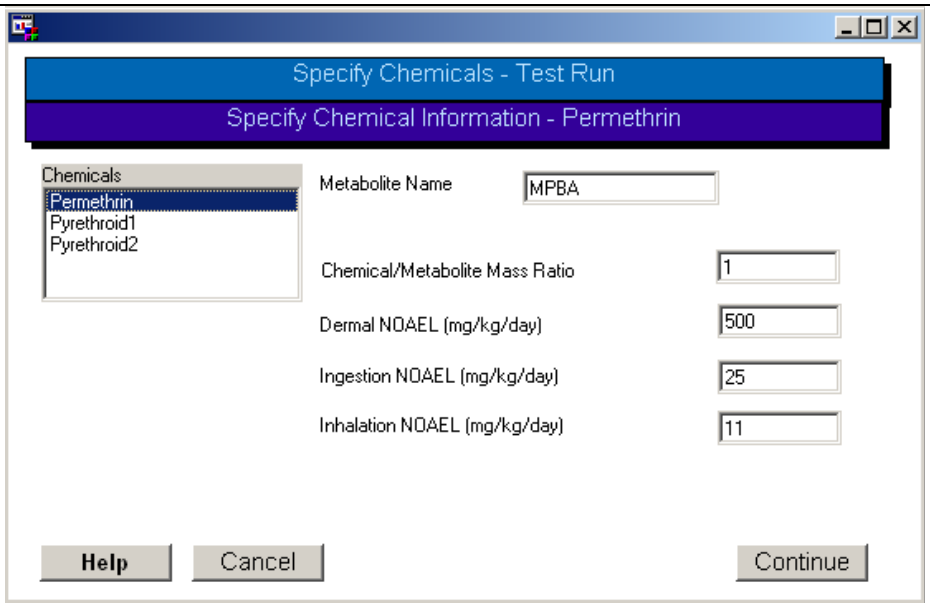


Figure 5.16. Specify Chemical Information Screen.

5.7 Specify Application Scenarios Simulated

Clicking on "Specify Application Scenarios" on the main screen begins a series of screens through which the user must navigate in their entirety before returning to the main screen. The exact screens vary depending on options selected. See Figure 2.1 for an overview of the screens in this section. The following screens may be visited:

The first screen is used to identify the scenarios to be simulated.

Specify Application Scenarios - Select Scenarios (Figure 5.17**)**

The second screen is used to specify details for each scenario and is used to get to the Application Dates and Co-Occurrence screens for each scenario.

Specify Application Scenario Details (Figure 5.19)

These screens are visited once for each scenario, after which the user is returned to the Specify Exposure Scenario Details screen:

Specify Chemicals in Scenario. (Figure 5.20). This screen only available when SHEDS in being run in cumulative mode.

Specify Application Dates (Figure 5.21 and Figure 5.22. The version visited depends on whether user-specified or model-determined application dates are being used.)

Specify Co-Occurrence (Figure 5.23. Only available when model-determined application dates are being used.)

Clicking the Continue button on the Specify Application Scenario Details screen takes the user to these screens. They are visited once for each simulation.

Specify Application Times (Figure 5.24. Only visited when model-determined application dates are used.)

Specify Fraction of House Treated for Indoor Scenarios (Figure 5.25)

Specify Re-entry Times (Figure 5.26**)**

5.7.1 Specify Application Scenarios

The specific scenarios or applications to be simulated are specified on this screen (Figure 5.17). In the later screens, additional information will need to be entered for each scenario defining the probability, dates, and co-occurrence of applications, fraction of indoor area treated, and re-entry times. The exact screens visited will depend on options chosen by the user. If the user is becoming familiar with the interface, it is recommended that only one or two scenarios be chosen.

This screen will not be shown (the button on the main screen will be grayed out) if the User-Specified Time Series was chosen as the source-to-concentration method. If the user is simulating a multimedia measurements study then specific applications are not specified.

Each scenario chosen is assigned a priority. The priority becomes important when application co-occurrence is of interest. That is, when one is interested in using the dates of one scenarios' applications to influence the dates of applications in other scenarios. The dates of an application can only be influenced by applications occurring in scenarios given a higher priority.

There are nine pre-defined application scenarios available in SHEDS. These appear in the Scenario Library. The available scenarios and their locations are as follows:

- **Lawn (Granular-Push Spreader).** Outdoor, Lawn.
- **Lawn (Liquid-Hand Wand).** Outdoor, Lawn.
- **Vegetable Garden (Dust, Powder).** Outdoor, Garden.
- **Indoor Crack and Crevice (Aerosol).** Indoor.
- **Indoor Crack and Crevice (Liquid).** Indoor.

- **Indoor Flying Insect Killer (Aerosol).** Indoor.
- **Indoor Fogger (Broadcast).** Indoor.
- **Pet Treatment (Spot-On).** Pet.
- **Pet Treatment (Liquid).** Pet.

The location of the scenario determines the exposure equations that are used, and thus the appearance of future screens and the information the user must supply for each scenario. (See the SHEDS Technical Manual for details of the exposure calculations). In addition to these built-in scenarios, the users can also add their own scenarios to the run (see next section).

Clicking on an application in the Scenario Library list box copies it to the list of "Selected Scenarios" in the middle of the screen. The scenarios are prioritized from top (1st) to bottom in the Selected Scenarios list. Click on a scenario description to select it. Use the up and down arrows on the right to change the priority of the selected scenario. Clicking on the "Delete Selection" button will delete the currently selected scenario from the Selected Scenarios list. When all desired scenarios are selected and prioritized, clicking on the Continue button will take the user to the remaining screens.

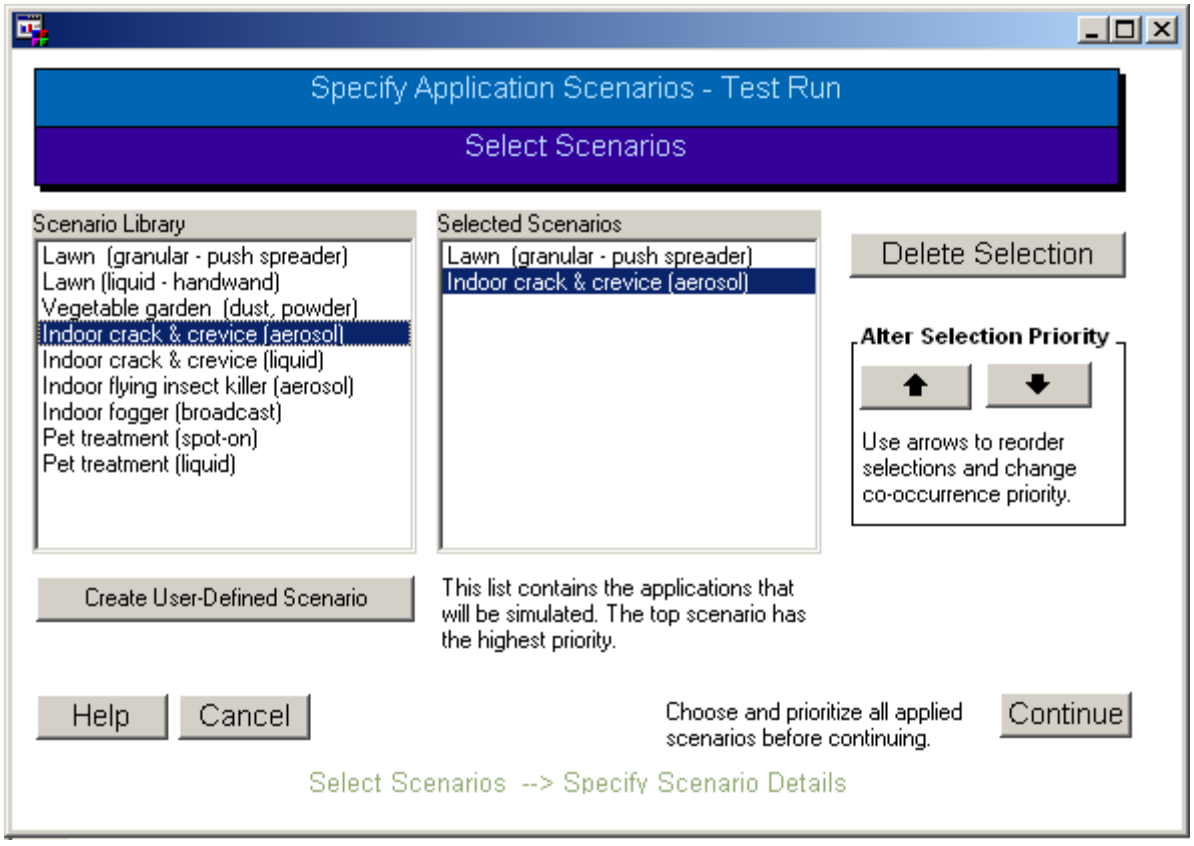


Figure 5.17. Specify Application Scenarios – Select Scenarios Screen.

5.7.1.1 Create User-Defined Scenario

SHEDS version 4 allows the users the option of adding their own custom scenarios to a run. This is accomplished by clicking on the "Create User-Defined Scenario" button on the Application Scenarios screen. This brings up the Add New Scenario screen (Figure 5.18). The user gives their scenario a name and a location, and clicks Add Scenario. The name given to the scenario will identify it on future screens. The location will determine the exposure equations that will be used for the scenario, and thus the appearance of future screens related to the scenario. The new scenario will be added to the Scenario Library on the previous screen, and the user can then add it to their run.

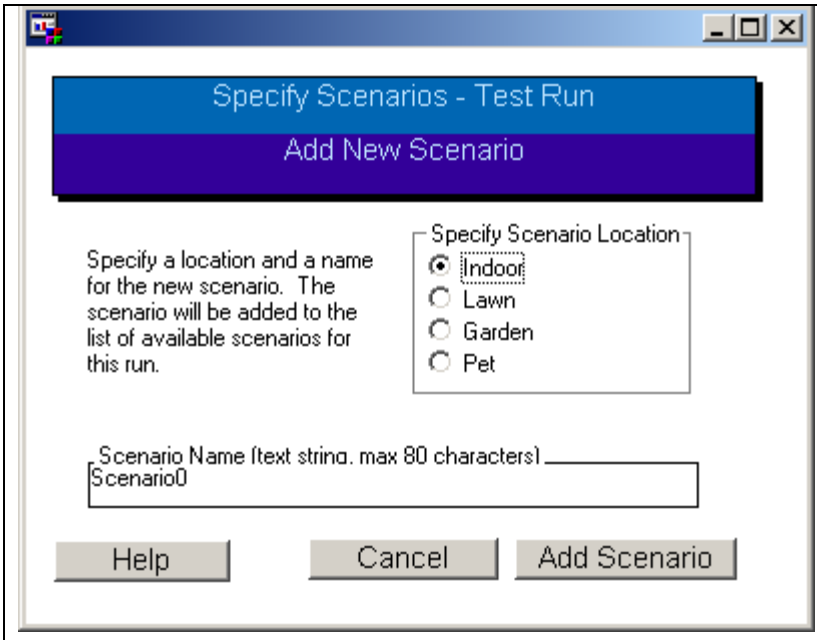


Figure 5.18. Add New Scenario Screen.

5.7.2 Specify Exposure Scenario Details

Once all application scenarios for a run have been selected, the user proceeds to the Specify Exposure Scenario Details screen (Figure 5.19) by clicking the "Continue" button on the previous screen. The list box on the left of this screen, labeled "Scenario", displays the scenarios chosen by the user in the previous screen. Clicking on one of these entries selects that scenario as the current one (and highlights it). Once selected, the user needs to do the following for each scenario:

1. Specify or edit the application probability.
2. Specify whether co-occurrence will influence this scenario's dates (not active for the scenario that is first in the priority list).
3. Click the Specify Inputs button to proceed to screens to enter application dates, times, and co-occurrence.

Only when these items have been completed for each scenario will the user be permitted to continue. If the existing values for probability and co-occurrence are acceptable, the user is not required to edit these values.

When using model-determined dates, the scenario's probability and co-occurrence status are displayed. The Application Probability is the probability that this application will be used by an individual that meets any requirement for usage (e.g., the person must have a garden for a garden application to occur). If user-specified dates are being used, this information is not required, because in that case the user directly specifies the dates of application for each scenario, and this presupposes that the simulated population is restricted to those who can apply the specified scenarios.

When simulating product handlers, a Probability of Being a Handler entry box is visible. The user enters the probability that each profile meeting the age requirement is a handler. For example, if the user has previously specified that the minimum age for handlers is 16 years, this probability determines how many of the simulated profiles age 16 or greater are handlers. If handlers are not included in the run (see Section 5.5.5) then this entry box will not be present.

Even when model-determined dates are being used, the "Specify Co-Occurrence" radio box will be grayed out for the application with the highest priority since no other scenarios are allowed to influence it. If co-occurrence is active, the user may select either No Co-occurrence or Specify Parameters in the "Scenario Co-Occurrence" radio box. If Specify Parameters is selected, then the application dates of other scenarios will be allowed to influence the application dates of this scenario. Selecting this here will cause the "Specify Co-Occurrence" screen to be displayed at the appropriate time.

Once the application, handler, and co-occurrence information is entered for a particular scenario, the user may click on the "Specify Inputs" button to proceed to the Specify Chemicals, Specify Application Dates and Specify Co-Occurrence screens for that scenario (see next sections). After completing the information on these screens the user will be returned to this screen to work on the remaining scenarios.

Scenarios that have been completed are shown in the list box on the right. The user will not be allowed to continue (click on the Continue button) until the application date and co-occurrence information has been filled out for all selected scenarios. Clicking on the Continue button will take the user to the Specify Re-entry Times and possibly the Specify Application Times screens.

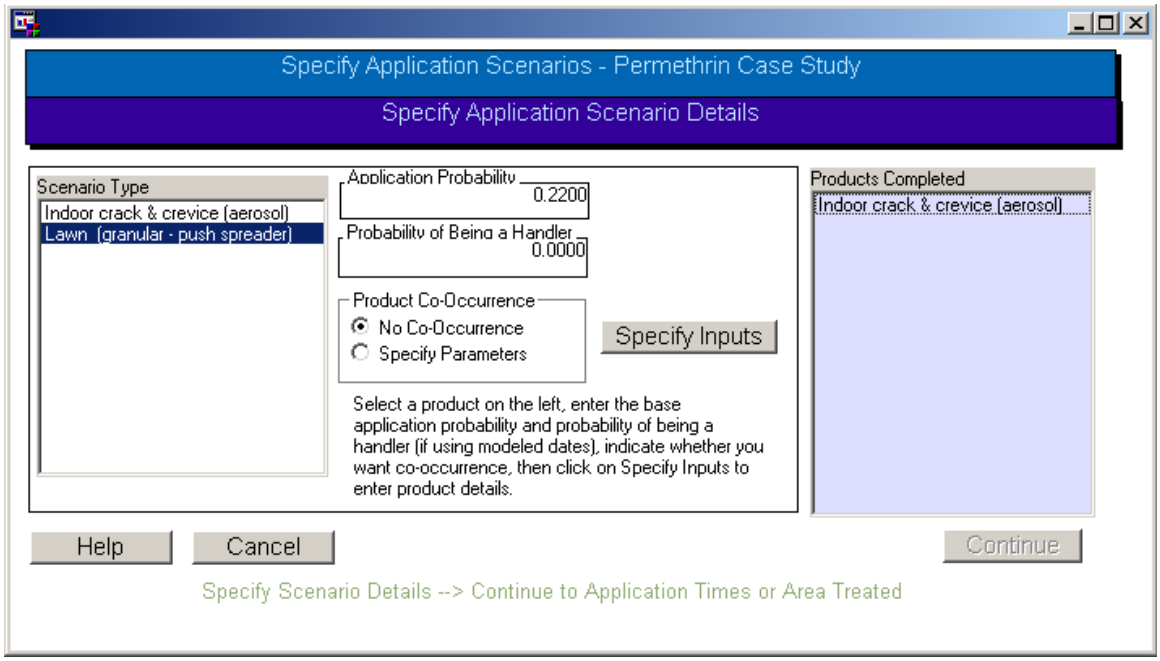


Figure 5.19. Specify Application Scenario Details Screen.

5.7.3 Specify Chemicals in Scenario

In SHEDS, not all chemicals in a run need be present in all scenarios. In this screen (Figure 5.20) the user specifies which of the chemicals included in the simulation are present in the current scenario. At least one chemical must be present in the scenario, (otherwise, the scenario should not be included in the run since it has no influence on exposure). If SHEDS is being run in Aggregate mode, this screen will not appear, as it will be assumed that the single chemical being studied is present in all scenarios. If a single-chemical run is being performed in Cumulative mode, the user will visit this screen but only one chemical will be available for selection.

The user selects the chemicals for the current scenario (the name of which will be included on the third header bar) by simply clicking in the Chemicals selection box. The user can remove a previously selected chemical via the Delete Selection button.

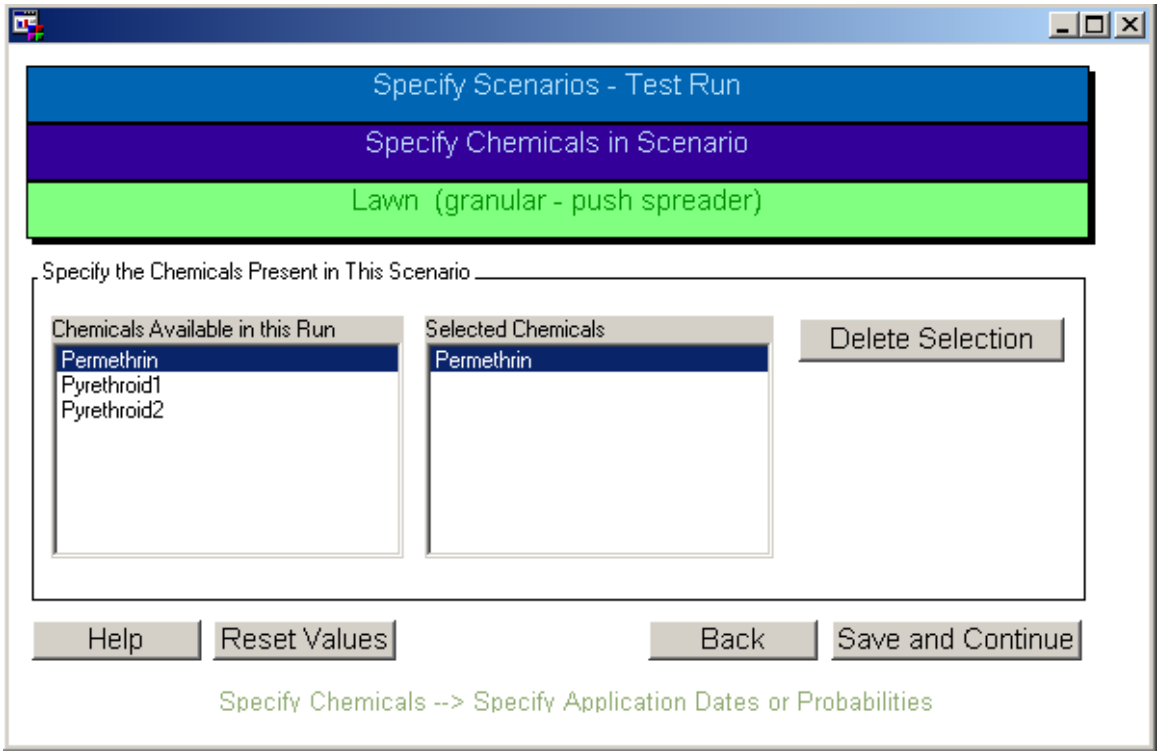


Figure 5.20. Specify Chemicals in Scenario Screen.

5.7.4 Specify Application Dates: Model-Determined

If model-determined application dates are being used, the Specify Application Dates screen appears as in Figure 5.21. Model-determined dates are determined stochastically during the simulation. The dates will typically vary for each individual simulated. The user enters the blackout period, the probability vectors for month, day of week, and number of applications. These are used together to determine randomly the application date or dates for each person. During a simulation the actual dates chosen may be influenced by other scenarios if co-occurrence was specified.

Taken together, the probabilities define the likelihood of an application occurring on each day of the year. For multiple applications the blackout period comes into play. The blackout days indicate how many days must pass before an additional similar application is allowed.

The probabilities for each vector (weekday, monthly, and number of applications) must total 1.0. The user can enter probabilities in the first boxes of each probability vector. The last box of the vector, with a darker border, will always contain the remainder and cannot be edited by the user. Additional information about entering probability vectors is given in the section “Entering Probability Vectors” on page 9.

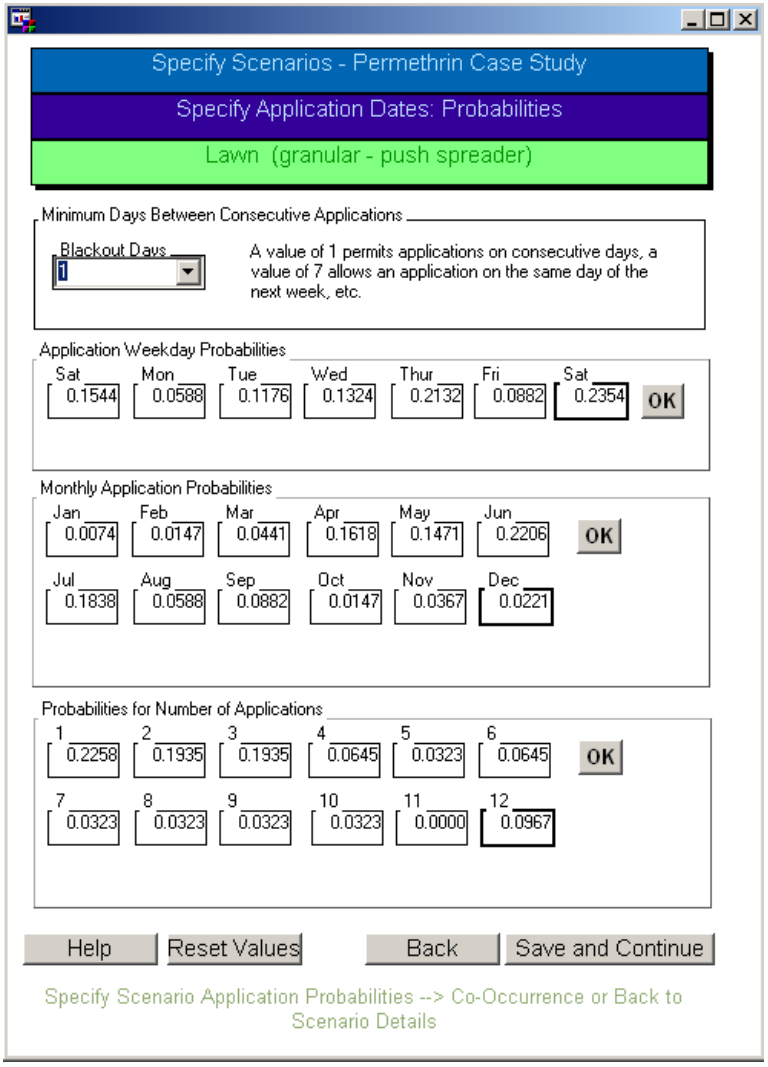


Figure 5.21. Specify Application Dates Screen for Model-Determined Application Dates.

5.7.5 Specify Application Dates: User Specified

This screen (Figure 5.22) is used to enter application dates when the "user-specified dates" option is selected (see Section 5.5.2). These dates are specified by day number (with 1 being the first day of the simulation period). There is no probability associated with these application dates, as an application will be made on each of these dates for all persons in the run. In addition to the days of application, the user should select the time. All applications in a scenario will be made at the same time of day.

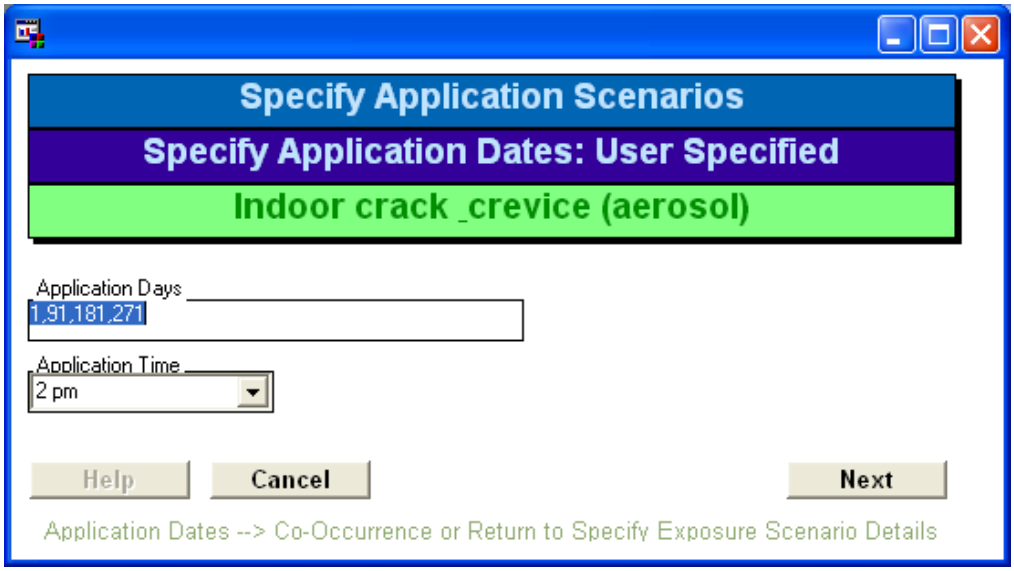


Figure 5.22. Specify Application Dates: User Specifed Screen.

5.7.6 Specify Co-Occurrence

This screen (Figure 5.23) is used to specify how the application dates of other scenarios affect the application dates of this scenario. Scenarios must have been specified as being of a higher priority in the Specify Exposure Scenarios screen to affect a scenario. Only those scenarios of a higher priority are listed in "Application Types of Influence". For purposes of discussion let us call the scenario we are working with the "current" scenario, and let us call applications from scenarios with higher priority "previous" applications. In the model code, the dates of the previous applications will be determined first. Here "previous" refers to the order in which the application dates are determined; these do not necessarily occur earlier in the simulation.

Note: Co-occurrence can only be selected in SHEDS if the chemical application dates are model-determined. If user-specified chemical application dates are selected in the Simulation Information Screen, then the co-occurrence will be disabled.

The probability of an application from the current scenario occurring on any day of the year is determined based on the probability vectors entered earlier for month and day of week. When working on the current scenario, the application dates for the higher priority scenarios will already have been determined. The probabilities for the current scenario are altered (multiplied) by the influence factor for all days within the influence width of previous applications. This obviously has no effect for those days whose probability is already 0. The influence factor, also called the co-occurrence probability is discussed and illustrated in the "Application Dates and Co-occurrence" section of the Technical Manual.

If the influence factor exceeds one, then the likelihood of the current scenario happening near in time to a previous scenario is increased. If the influence factor is less than one, the likelihood is decreased. An influence factor of zero means that a 'blackout window' is created around each of the dates for the previous scenarios, so that the current scenario cannot occur on those dates. The two scenarios become mutually exclusive for that period of time around an application.

The user must choose an effective combination to continue. That is, at least one application type must be highlighted and the influence factor must be different from 1. If the user wants to turn off co-occurrence for this scenario, then enter an effective combination and return to the Specify Scenario Details screen. On that screen click the No Co-Occurrence choice for this scenario. This will turn off co-occurrence.

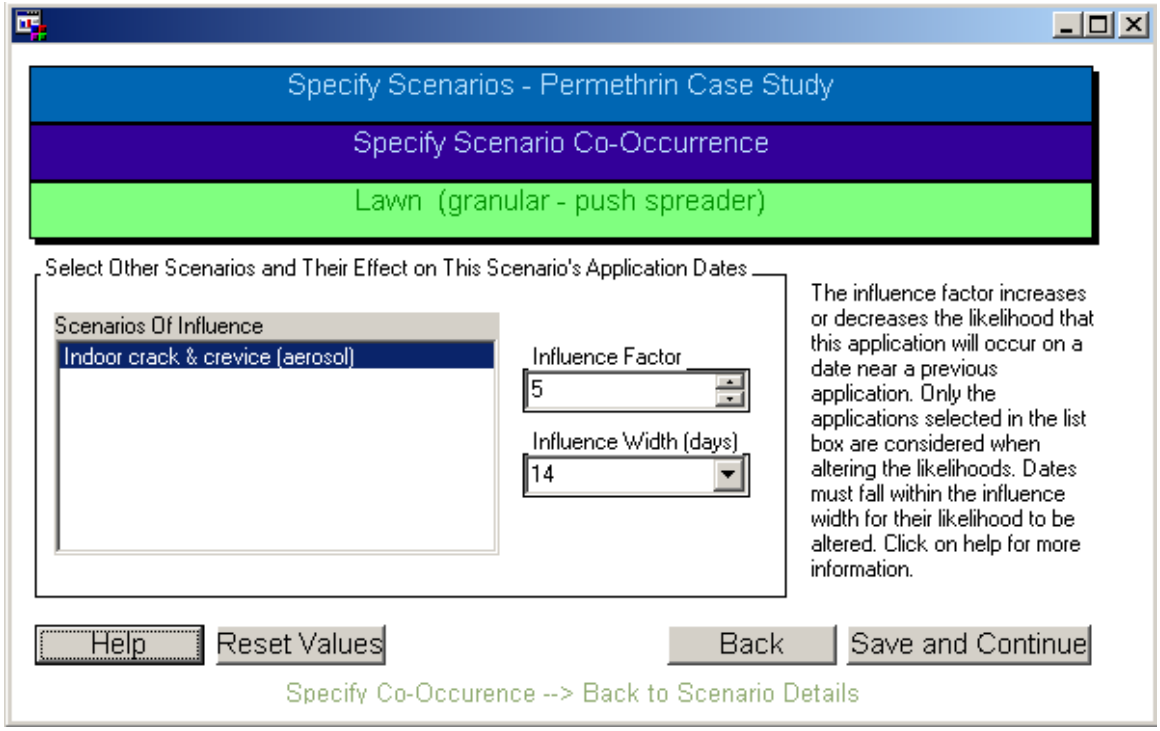


Figure 5.23. Specify Co-Occurrence Screen.

5.7.7 Specify Application Times

When model-determined dates are specified, the user will also need to specify probability vectors for the application times. This screen (Figure 5.24) allows the user to enter one probability vector for all applications occurring inside, one probability vector for all applications occurring outdoors, and one for all pet applications. If the current run does not contain scenarios in one of these locations (indoors, outdoors, or pet), then the corresponding vector will not be visible. For a fixed application time for each simulated individual simply enter a probability of 1 in the appropriate box. For general information on entering data in probability vectors see the section "Entering Probability Vectors" on page 9.

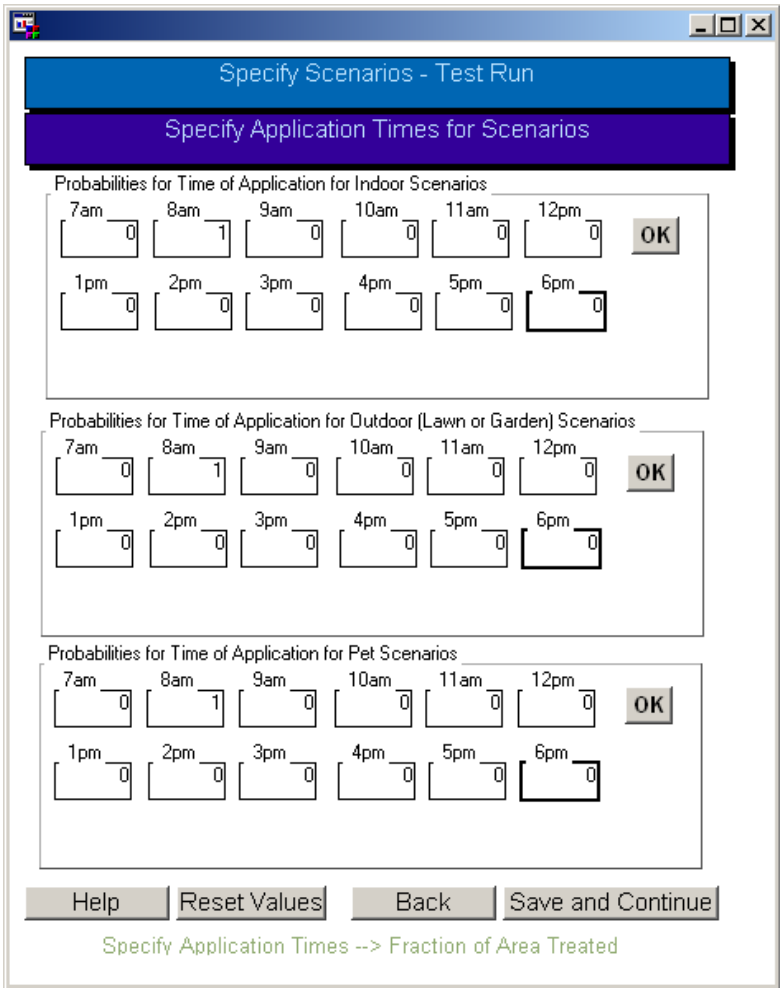


Figure 5.24. Specify Application Times Screen.

5.7.8 Specify Fraction of Area Treated

For indoor scenarios, SHEDS requires the user to enter the fraction of the house being treated (Figure 5.25). See the Technical Manual for how this information is used in the exposure calculation. The indoor scenarios included in the current run will be listed in the list box on the left side of the screen; the user selects each of these in turn and enters the distribution for the variable. For general information on entering data in distributions see Section 2.3.5.

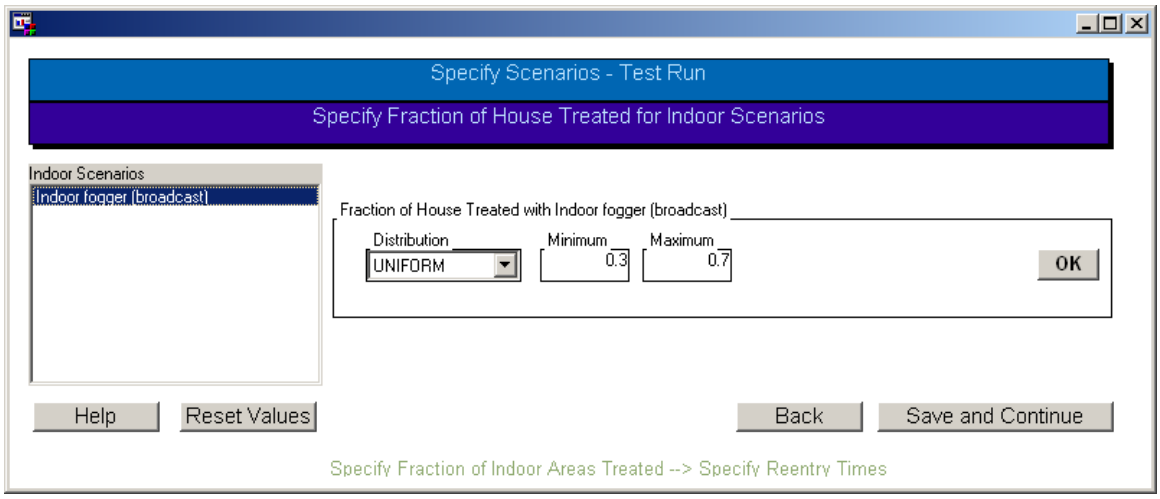


Figure 5.25. Specify Fraction of Area Treated Screen.

5.7.9 Specify Re-entry Times

Simulated individuals may be restricted from entering treated areas for a specified number of hours. This restriction is split into reentry times for indoor areas and outdoor areas, and a ban time for contact with pet. If scenarios for any of these locations are not present in the current simulation, the distributions for the location will not be present (for example, if there are no pet scenarios in the run, the ban time on contact with pet distribution will not be visible.) Within each area the probability of re-entry is the same for all scenarios affecting that area. The probabilities are entered on the Specify Re-entry Times screen (Figure 5.26). For general information on entering data in distributions see Section 2.3.5.

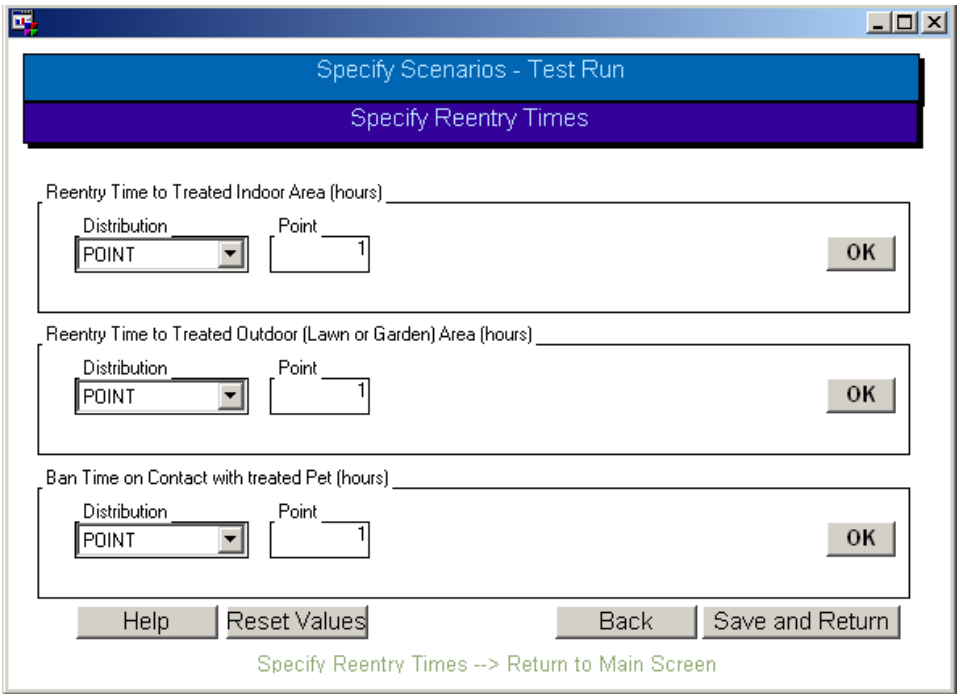


Figure 5.26. Specify Re-entry Times Screen

5.8 Specify Concentration-Related Inputs

Clicking on "Specify Concentration-Related Inputs" from the main screen begins a series of screens through which the user must navigate in their entirety. The exact screens vary depending on the source-to-concentration options selected earlier. Since these screens may have to be revisited for each scenario, the scenario being edited is always displayed in the third (blue) title at the top of the screen. These screens are also chemical-dependent, so a chemical selection widget is also present on each screen.

WARNING: Different surface residue collection devices are available (e.g., aluminum plates, rollers, sleds, hand presses, hand wipes); some collect dislodgeable residues and some collect total residues. These methods, as well as current methods for obtaining dermal transfer efficiencies and dermal transfer coefficients, have inherent uncertainties. Thus, it is important to consider matching the correct type of surface loading with the corresponding transfer factor (i.e., transfer efficiency or transfer coefficient) when developing inputs for modeling dermal exposure.

Please see the technical manual (section on Dermal Exposure to Surface Residues) for a discussion of entering compatible concentrations and transfer factors (e.g., to prevent double counting of residue transfer from surfaces to skin).

The following screens will be visited once for each scenario selected, depending on the overall method used. The exception is the Background screen which is only visited once.

Decay and Dispersion: **Specify Decay and Dispersion Distributions (**Figure 5.27**)**
Handler Distributions (if needed) (Figure 5.29**)**
Background Concentration Distributions(Figure 5.30**)**

Intervals: **Specify Interval Concentration Distributions (**Figure 5.28**)**
Handler Distributions (if needed) (Figure 5.29**)**
Background Concentration Distributions (Figure 5.30**)**

The Time-Series option only requires a single input in this section:

Time series: **Specify Time Series Input (**Figure 5.31**)**

5.8.1 Specify Decay and Dispersion Distributions

Use of the decay and dispersion method requires that a number of distributions be defined for each scenario. These distributions define the initial media concentrations and the decay rate of the chemical for the current scenario. Additionally, for indoor scenarios the rate of dispersion to the untreated part of the house must be calculated. To do this, SHEDS requires as input a distribution for the untreated to treated area concentration ratios. (See the Technical Manual for more details.) If the user chooses to ignore dispersion into the untreated area, then this ratio should be set to a point value of zero.

The following are the required distributions for each type of scenario:

- **Indoor Scenarios**
  - Concentration in indoor air immediately after application
  - Concentration in indoor air 24 hours post-application
  - Initial concentration on carpet
  - Initial concentration on hard floors
  - Initial concentration in dust
  - Chemical decay rate
  - Ratio of treated to untreated indoor room concentrations

- **Lawn Scenarios**
  - Initial concentration on the lawn
  - Initial concentration in the lawn soil
  - Chemical decay rate

- **Garden Scenarios**
  - Initial concentration on the garden
  - Initial concentration in the garden soil
  - Chemical decay rate

- **Pet Scenarios**
  - Initial concentration on the pet
  - Chemical decay rate

There will be one distribution entry widget for each of these scenarios. All this information must be entered for each chemical. The user selects the current chemical from the list on the left of the screen. The user will not be able to move to a new chemical if errors are present in the data for the current chemical.

General information on distributions are provided in section “Distributions Supported” on page 11 and information on entering distributions on this screen are discussed in “Individual Distribution Widgets” on page 11.

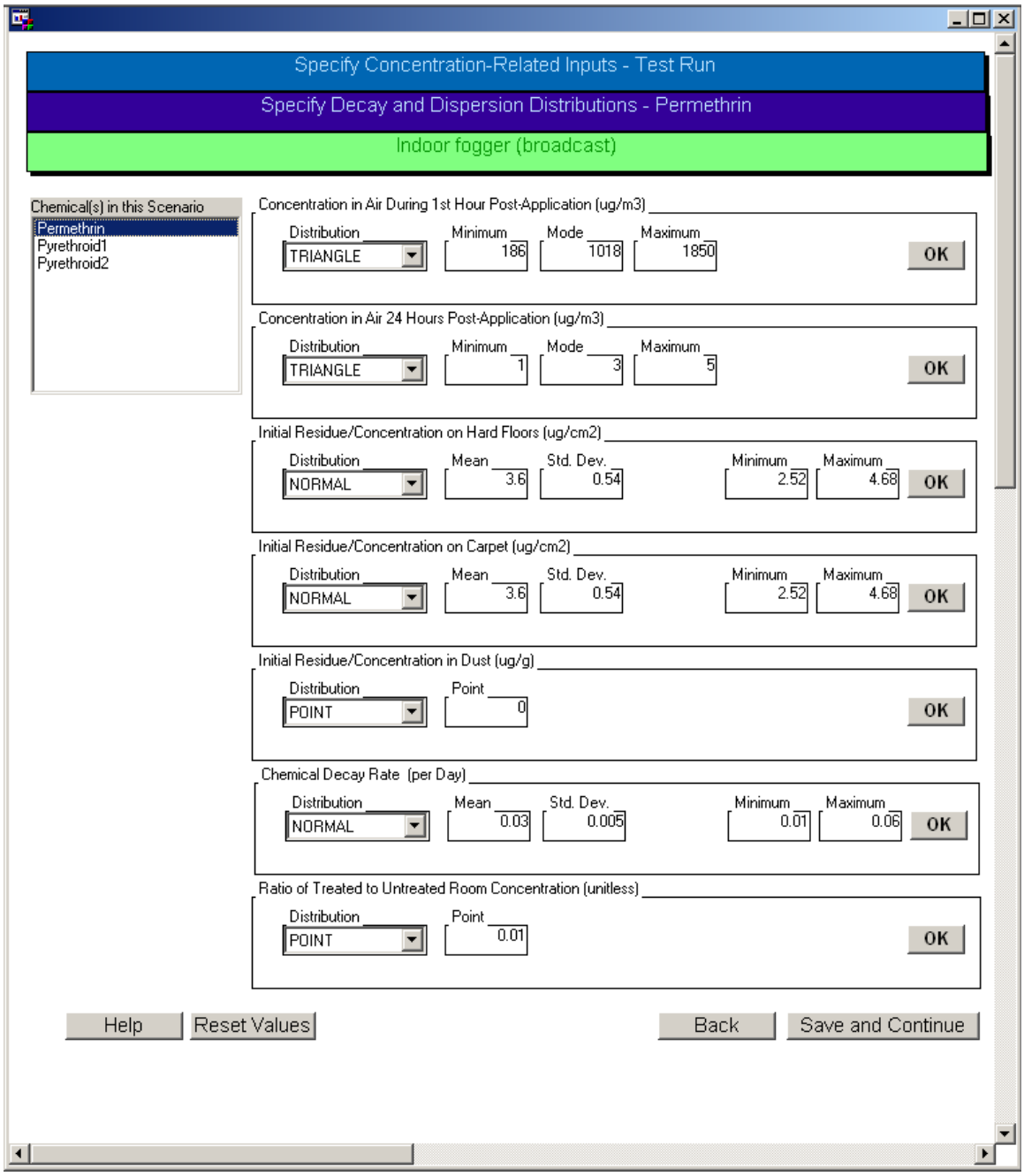


Figure 5.27. Specify Decay and Dispersion Distributions for an Indoor Scenario.

5.8.2 Specify Interval Distributions

Interval distributions might be used when measurement studies have determined the actual concentrations over time after applications. SHEDS uses four time periods:

1. The day of application (< 1 day)
2. The day after application to 7 days after application (1-7 days)
3. The 8th day after application to the 30th day (8-30 days)
4. The 31st day after application and the remainder of the simulation period.

The user must define these four distributions for each medium affected by each scenario for each chemical. Once an application is made for a scenario, these distributions will determine the concentrations on each medium. When another application is made in the same scenario, the first distribution is used once again; there is no persistence of chemical from the previous application. The concentrations on a medium from different scenarios are added when determining exposure of an individual. It is assumed that background values are included in the distributions; the user cannot define background concentrations on media not included in the scenarios.

As on the previous screens, the third title, in blue, indicates the current scenario. Clicking on a medium/chemical combination in the Interval Variable list box selects and highlights that variable. The distributions displayed are related to that variable for the current scenario. The user is not forced to enter data for each combination. Any distributions not entered by the user will retain their previous values whether desirable or not. Once the distributions have been edited as desired, the user should click on Continue to go on to the next scenario. If this is the only or last scenario, then the next screen will be used to define background values.

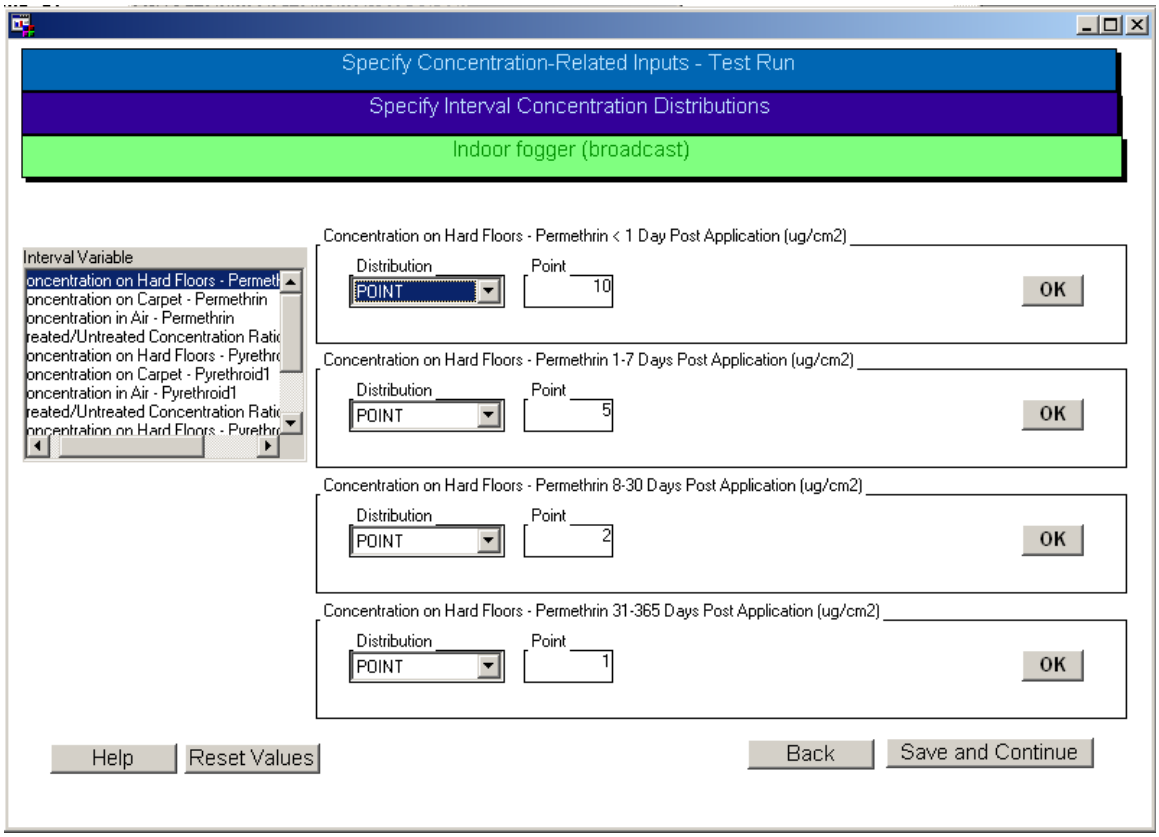


Figure 5.28. Specify Post-Application Distributions Screen for An Indoor Scenario

General information on distributions are provided in section “Distributions Supported” on page 11 and information on entering distributions on this screen are discussed in “Individual Distribution Widgets” on page 11.

5.8.3 Specify Handler Distributions

If handlers are being modeled, the following screen (Figure 5.29) appears for each scenario. On this screen the user must enter the following distributions:

- Application Rate of chemical being applied.
- Unit dermal exposure of the handlers.
- Unit Inhalation exposure of the handlers.

See the Technical Manual for details of the handler exposure calculations.

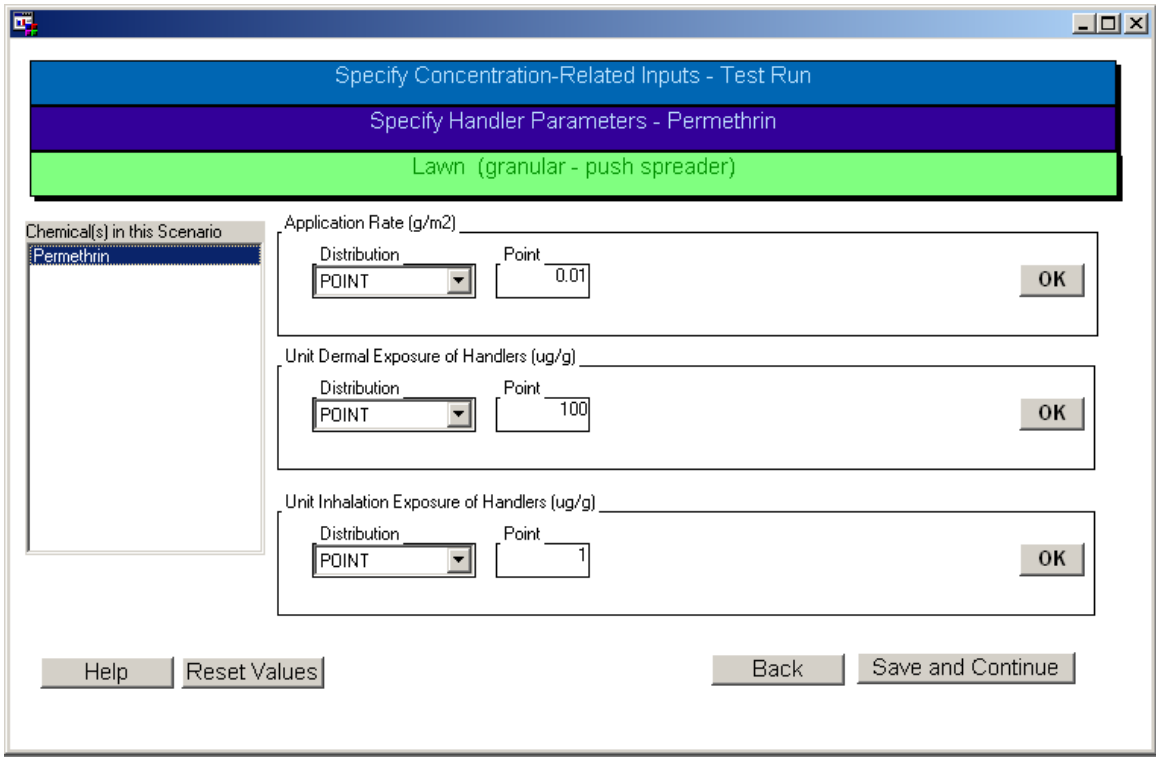


Figure 5.29. Specify Handler Distributions Screen

5.8.4 Background

A background screen (Figure 5.30) will be visited for both Decay and Dispersion and Interval Distribution options (the only difference will be the title on the middle header bar). On this screen the user must enter the background concentrations for outside surfaces. This is the only background concentration distribution required by the model. The concentration must be entered for each of the chemicals in the via the Chemical selection list box on the left side of the screen. The user will not be able to move to a new chemical if there is an error in the data for the current chemical.

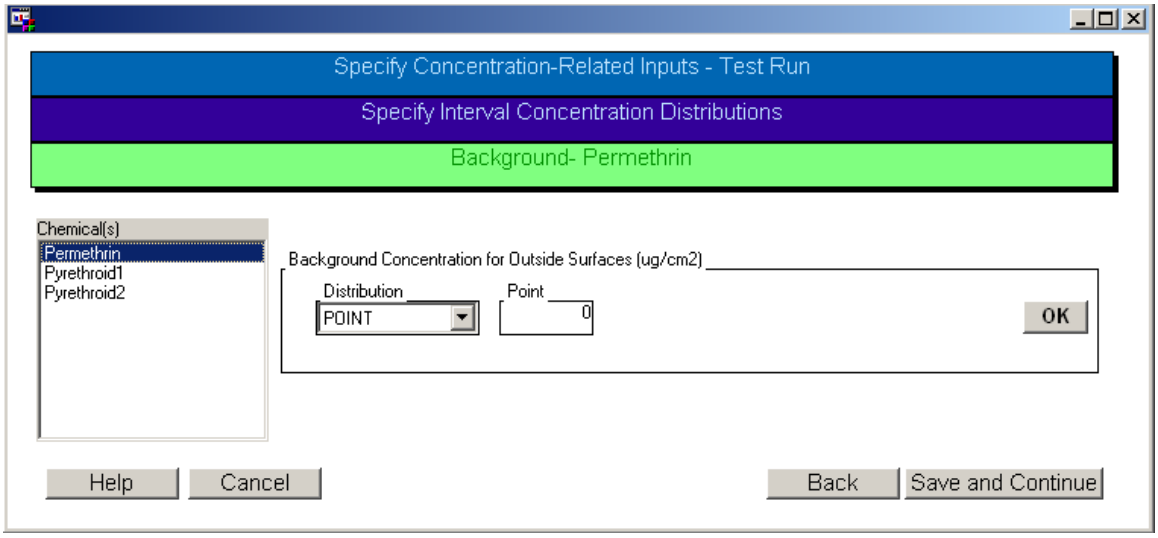


Figure 5.30. Background Screen.

5.8.5 Specify Time Series Inputs

Time series inputs allow the user to specify the exact concentrations on each medium for specific dates. This is a convenient method of using data derived from studies of multiple households. Details on the file format required are discussed in the SHEDS Technical Manual.

The burden is on the user to create the file containing time series for all affected media. The interface expects to be given a single SAS dataset which is copied into the input directory for the run. The dataset is specified by clicking on Copy Time Series Dataset (Figure 5.31) and then using the explorer to identify the dataset.

When using time series inputs the Specify Application Scenarios button on the main screen is grayed out. The model does not simulate specific applications in this case.

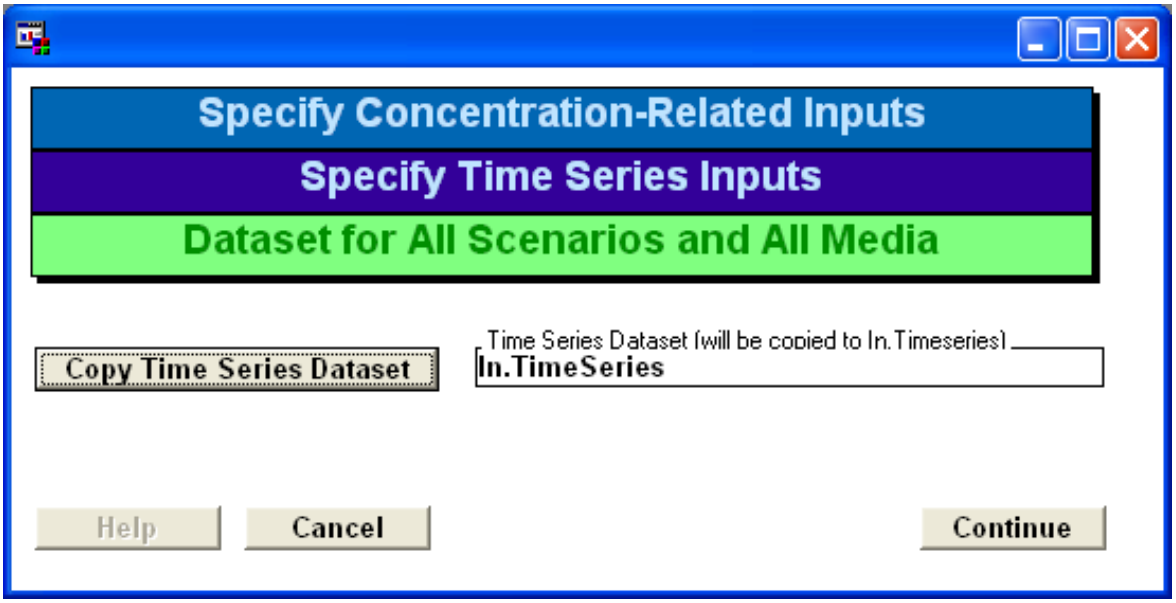


Figure 5.31. Specify Time Series Inputs Screen.

5.9 Specify General Exposure and Dose Factors

Clicking this button on the main screen begins a sequence of screens allowing the user to enter or edit the remaining inputs. These inputs fall into two broad categories:

1. Individual exposure and dose factor variables, typically defined by a distribution.
2. Correlation between input variables (optional).

Each of these categories is discussed in the sections below.

Initially the user is taken to the **Variability Distributions** screen (Figure 5.32). From this screen the user repeatedly visits the **Edit Variability Distribution**s screen (Figure 5.33).

If the user desires to define correlated inputs, clicking on Define Correlated Input Variables will lead to the following two screens: **Select Correlated Variables** (Figure 5.37), and **Specify Variable Correlations** (Figure 5.40). The first "Select Correlated Variables" screen is used to select which variables are to be correlated; the "Specify" screen is used to specify the correlation values defined.

5.9.1 Variability Distributions

The variables set using the first two screens in this series are grouped as follows:

- Baths (time between baths).
- Dose-Related (GI and dermal absorption rate, elimination rate, etc.)
- Removal-Related (hand washing frequency, removal efficiencies, etc.)
- Transfer-Related (skin adherence, non-dietary ingestion, etc)
- Activity-Related (Probabilities related to lawns, gardens, and pets)

Each variable is defined by a distribution, except for the time between baths, which is a probability vector.

The initial Variability Distributions screen (Figure 5.32) is used as a jump point. The user selects a variable group by clicking on the group name in the Variable Groups list box. The group is highlighted and the descriptions of each variable in the group are displayed in the center list box. Clicking on the Specify Inputs button will take the user to the next screen where individual distributions can be edited. After clicking Continue (or "Save" for the Baths screen) , the user will be returned to this screen. The variable group just edited will be added to the Groups Completed list box if it was not already there. While one or more variable groups remain to be edited, the background of the Groups Completed list box will be light blue and both the Define Correlated Input Variables and the Continue button will be disabled. When all groups have been completed the user may continue contact distribution screens.

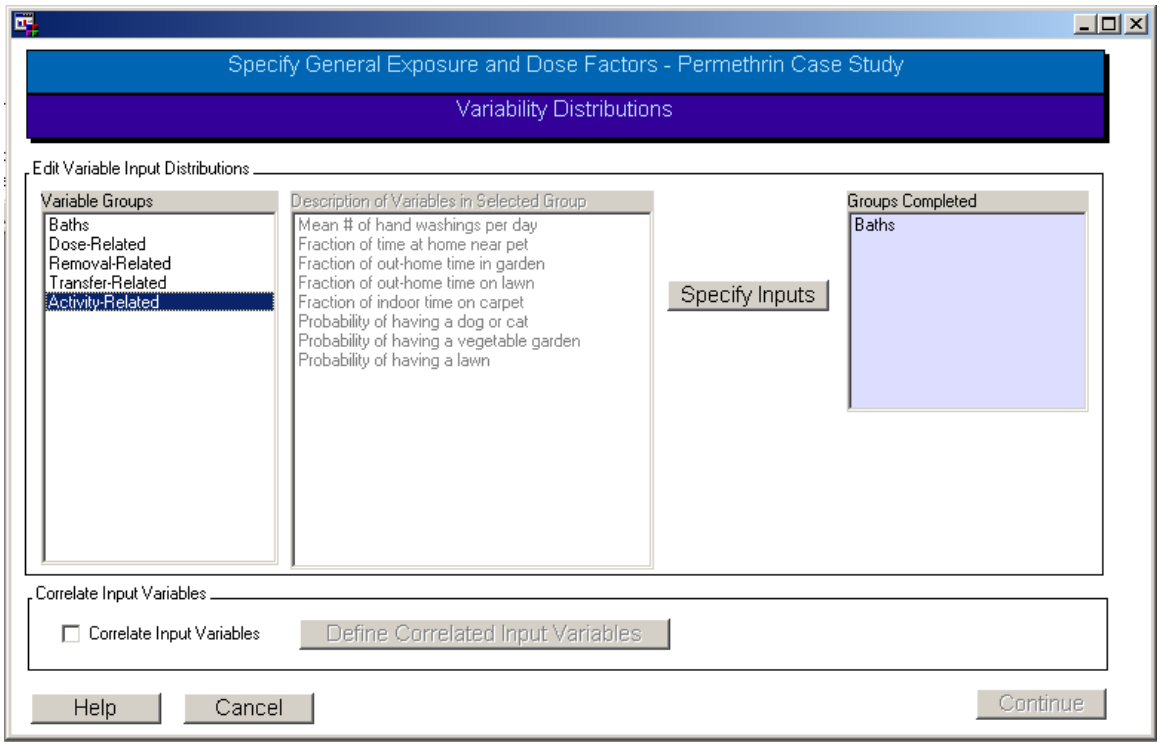


Figure 5.32. Variability Distributions Screen.

If the user returns to the Simulation Information screen and changes options, she will be forced to return here and enter values for any variables not previously defined. For example if the simulation options are switched to Transfer Coefficients from Transfer Efficiencies, the user will need to return here to edit the Transfer-Related group. Only then will the user be able to continue and run the simulation.

Once all groups are completed, the user will be able to define correlated inputs. By default, correlated inputs are turned off; no input variables are correlated. To turn correlation on, click on the check box labeled Correlate Input Variables. This will enable the Define Correlated input Variables button. Click on the button to proceed to the two screens used to select and define correlated inputs. After defining correlated inputs, the user will be returned to this screen. If the definition of correlated inputs is not completed, input correlation will be turned off when the user returns to this screen.

Only when all variable groups have been completed will the user be allowed to continue. If correlation was turned on, the correlated pairs must be defined or correlation must be turned off before the user may continue. Once enabled, clicking on the Continue button takes the user to the screens used to define contact probabilities.

5.9.2 Edit Variability Distributions

The user comes to this screen (Figure 5.33) when the Specify Inputs button is clicked from the Variability Distributions Screen. The screen will always have the same basic layout, but the specific variables that can be edited will change based on the variable group highlighted when the Specify Inputs button was clicked. The second title will always indicate the variable group being edited.

The variable to be edited is chosen in the left hand list box. If the variable has several distributions associated with it, for different ages perhaps, then a list of conditions will be listed on the right (see Figure 5.34). A variable is selected by Clicking on the variable description, or the condition if present. When selected, the current distribution parameters for that variable will be loaded into the widget. The title of the box surrounding the distribution widget will show the actual variable name, a vertical bar, and then the description for that variable. Use of the distribution widget is covered on page 12.

Whenever a valid distribution is loaded or redefined a frequency histogram will be drawn showing a representative sample for the distribution as defined. To turn this off, uncheck the histogram check box on the right. The mean and standard deviation of the sample will also be shown in the box on the right. It should be emphasized that the sample shown is not used in the model. The distribution will be sampled during the model run to generate values used in the run. Some features, particularly due to truncation, are easier to see if the number of bins are increased using the spin box on the right. If the current run is an uncertainty run (see Section 5.4), the "Uncertainty" distribution definition may be selected for any variable. (See section 2.3.5.3 for

information on defining uncertainty distributions). When an uncertainty distribution is used, the user can view any of the distributions defined on the uncertainty dataset via a new widget labeled "Unc Distribution #" that will appear when "Uncertainty" is selected (Figure 5.35). By clicking the up and down arrows, the user can view any of the defined distributions.

The Print Plot button will route a copy of the plot to the default printer.

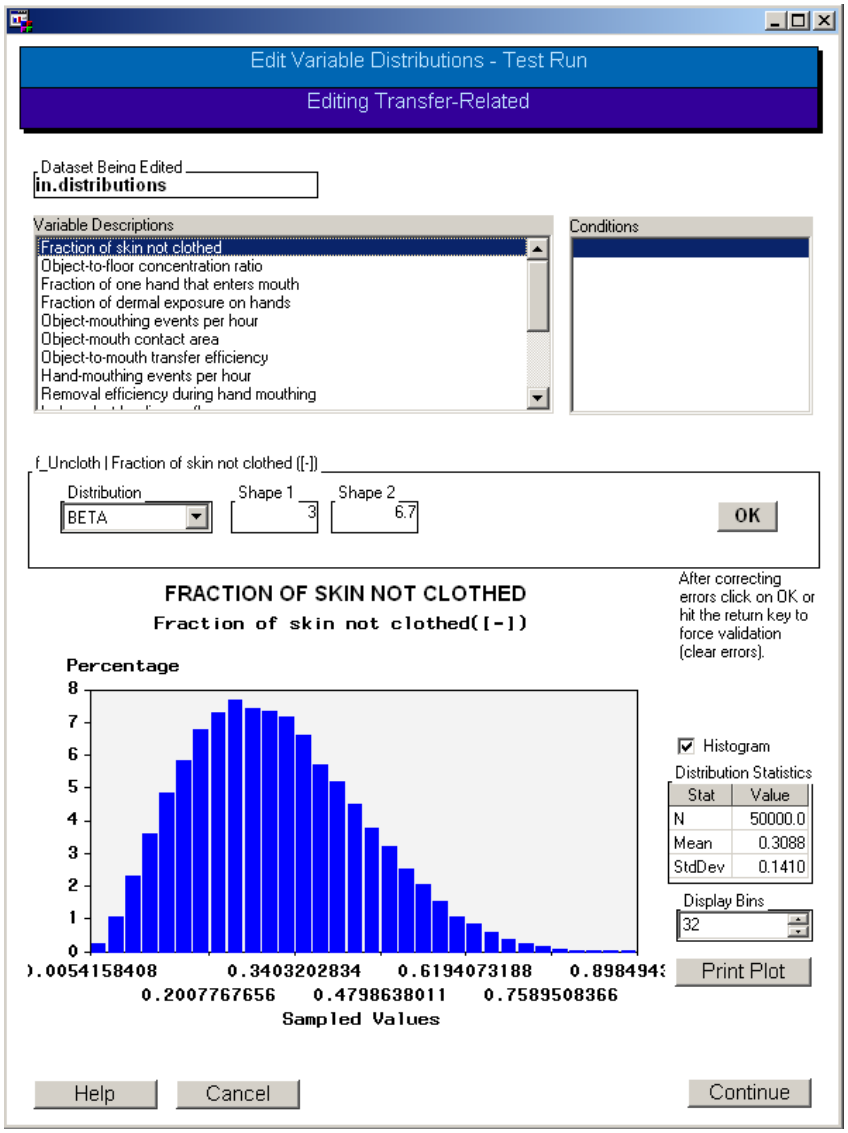


Figure 5.33. An example of the Edit Variability Distributions Screen for Transfer-Related Variables.

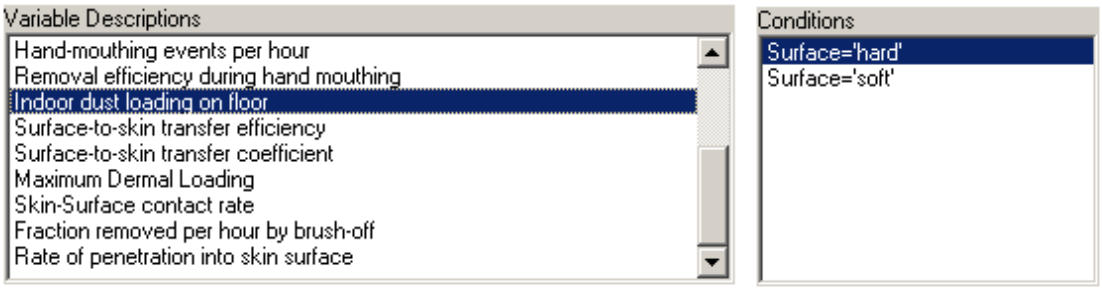


Figure 5.34. Variable with Two Conditions shown.

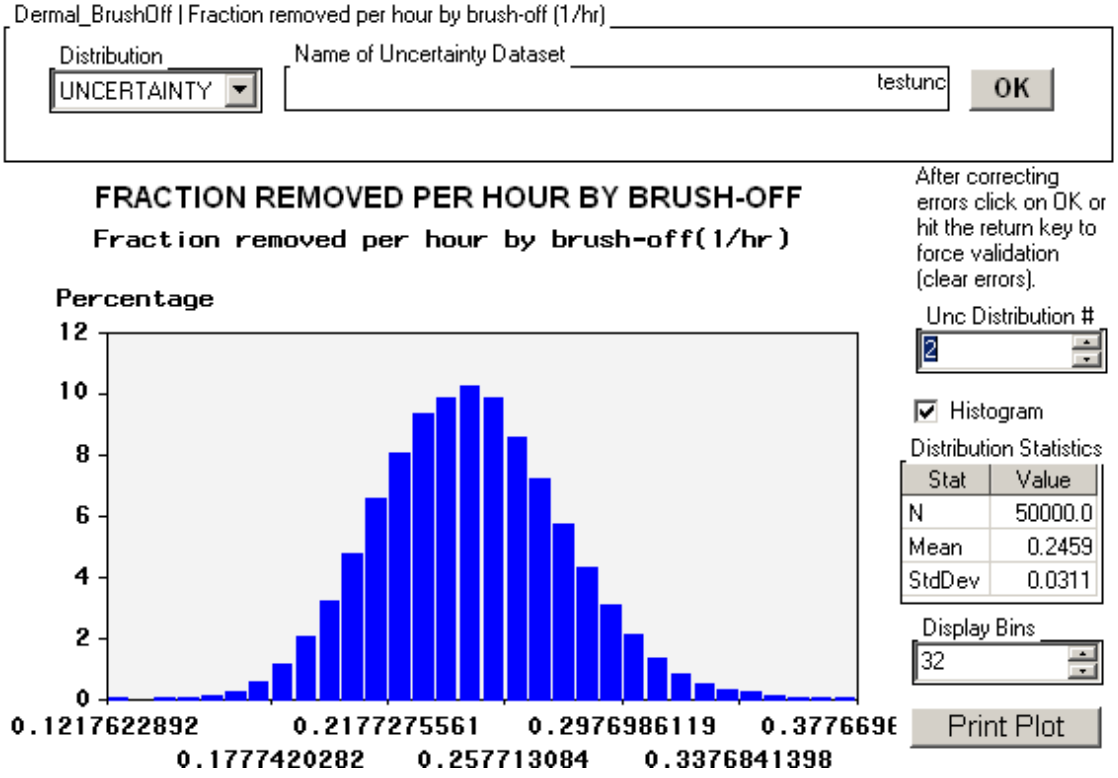


Figure 5.35. The Uncertainty Distribution # widget on the Edit Variability Distributions Screen when an Uncertainty distribution is Used.

To accept the current values, click the Continue button. If any of the parameter values are in error, they will be highlighted in red or yellow and the Continue button will be disabled. Clicking on the Cancel button returns the user to the Variability Distributions screen without saving any changes.

More detailed information on editing distributions is given in “Individual Distribution Widgets” in Section 2.3.5.

5.9.2.1 Days Between Baths

The Days Between Baths screen is a special case. When “baths” is selected from the Edit Variability Distributions screen, the specify Days Between Baths Screen (Figure 5.36) appears. On this screen the user enters the probability vector describing the distribution of days between baths for the population. See Section 2.3.3 for more information about entering probability vectors.

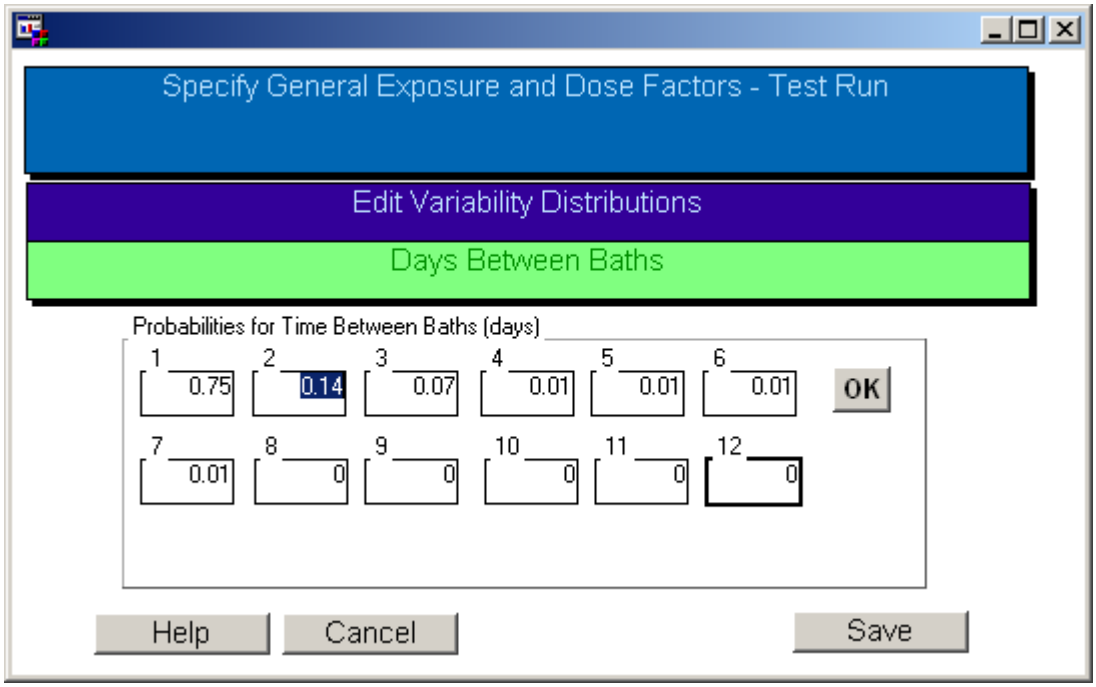


Figure 5.36. Specify Days Between Baths Screen.

5.9.3 Correlating Input Variables

All of the variables in this section (General Exposure and Dose Factors) are randomly sampled from the specified input distributions. In certain cases, the user might want some of these variables to be correlated with each other. For example, perhaps the hand-to-mouth transfer efficiency and the object-to-mouth transfer efficiency should have a tendency to track each other,

since the physical/chemical properties should be similar in both cases. This can be achieved in SHEDS by requesting that these inputs be correlated.

Any of the variables in the General Exposure and Dose Factors section (with the exception of probability vectors) may be correlated with others. The user selects the subset of input variables that will be subject to correlation, and then specifies the pair-wise Spearman correlations. If 'N' variables are selected for correlation, there are N(N-1)/2 distinct pairs. The user does not have to specify all pairs; any that are not given a definite target correlation are assumed to have a target correlation of zero.

SHEDS uses a modified NORTA[2] method to generate the correlations. The random values for the selected set of variables are first generated from a multivariate normal distribution with the correct Spearman correlations. Each normal variate is then transformed to the specified distribution using a rank-preserving transformation function. Since Spearman correlations depend only on rank, the Spearman correlations are preserved. The result is that the inputs will pair-wise exhibit the desired correlations, but will also have the marginal distributions requested by the user.

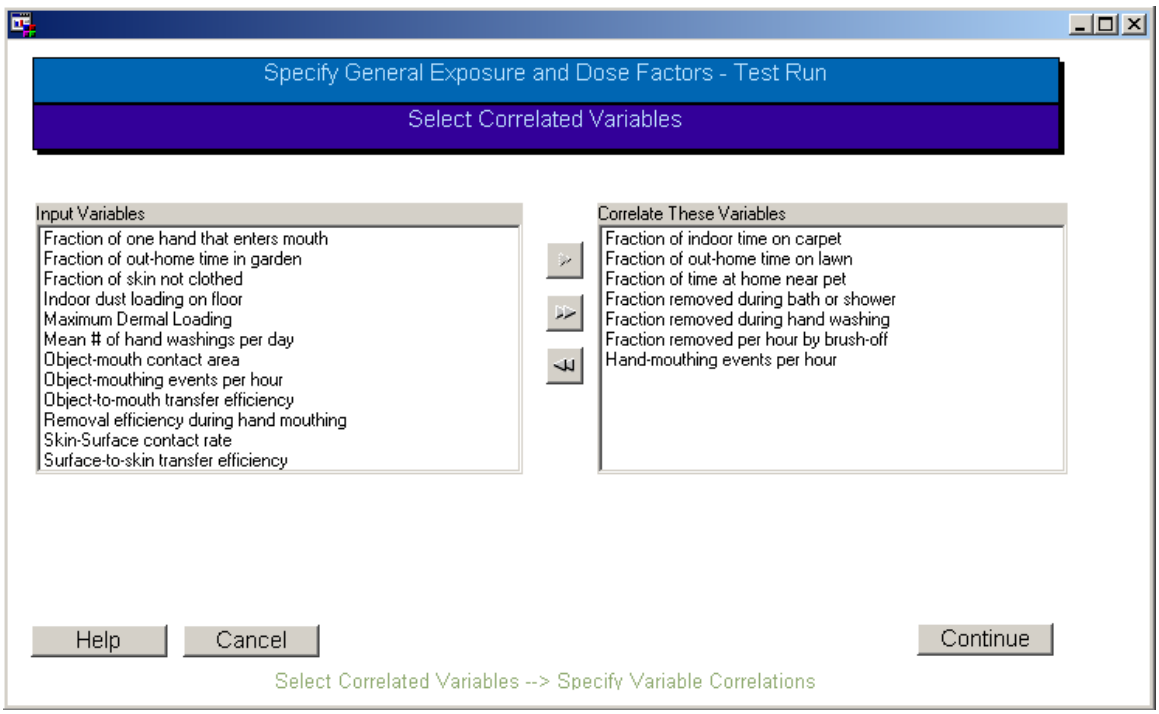


Figure 5.37. Select Correlated Variables Screen.

2 The NORTA method is described in the SHEDS technical manual.

It is possible to specify correlations that cannot be achieved. As an example, if two variables are to have a perfect correlation of 1.0, then each must have the same correlation as the other with any third variable. Mathematically, a correlation matrix is valid if and only if all its eigenvalues are non-negative. If the set of requested correlations is not allowed, a message is printed on the SAS log when the model is run.

Two screens are used to select and define the correlations. The first screen **Select Correlated Variables** (Figure 5.37) is used to choose the variables of interest. After choosing the variables, clicking on the Continue screen takes the user to **Specify Variable Correlations** (Figure 5.40) where specific pairs are assigned target correlation values.

5.9.3.1 Select Correlated Variables

The Select Correlated Variables screen (Figure 5.37) is used to choose which variables will be used to define correlated pairs in the next screen. It does not matter if variables are selected here which are not used later. Only valid variables will be displayed in the Input Variables list box.

Move variables to the Correlate These Variables list box to include them in correlated pairs on the next screen. The single arrow moves the selected variables, the double arrows move all variables. If the user has previously defined correlated pairs, the right hand list box will initially be populated only with variables in those correlated pairs.

Clicking on the Continue button will normally take the user to the Specify Variable Correlations screen. If the user selects less than two variables and clicks on Continue, an error will be displayed (Figure 5.38), correlation will be turned off, and the user will be returned to the Variability Distributions screen.

If no correlated pairs are chosen, then an error screen will be displayed (Figure 5.39), and correlation will be turned off in the simulation. Begin from the Variability Distributions screen to turn correlated inputs on once again.

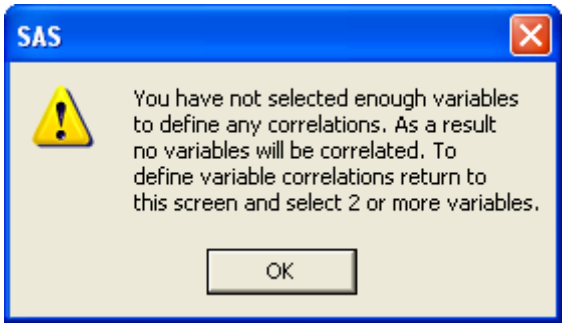


Figure 5.38. Error Displayed if Zero or One Variables are Selected for Correlation.

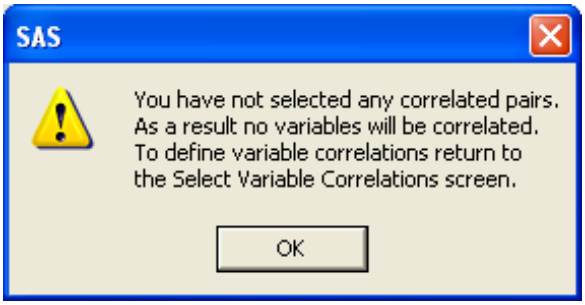


Figure 5.39. Error Displayed if No Variable Pairs are Selected for Correlation.

5.9.3.2 Specify Variable Correlations

This screen (Figure 5.40) is used to define or edit variable pairs and assign a correlation value to the pairs. A correlated pair is represented as two variable names and a correlation value from -1 to 1, inclusive. Note that the numbers in Figure 5.40 are hypothetical and for illustration purposes only; they are not intended to be recommended values.

The variables are ordered. Initially, all but the last variable are displayed in the First Variable list box. The Second Variable list box will contain all variables below the variable highlighted in the First Variable list box. The Second Variable list box will also always include the last variable.

The basic method of selecting a variable pair is to select the first variable in the First Variable list box, select the next variable from the Second Variable list box, specify the correlation value in the spin box to the right, and click on the Add Pair Button. Once added, the variable pair will be displayed in the Selected Pairs Specified box on the lower portion of the screen.

If a variable pair selected in the upper list boxes was previously specified and is already listed below, then the Add Pair button will not be enabled. Instead, the Replace Pair button is enabled and will replace the correlation value currently specified with the one previously specified for the pair.

The user may find it necessary to resize the columns in the Correlated Pairs Specified area. This area is capable of displaying both variables in the pair and the correlation value. Sometimes the columns are not initialized such that all three are visible.

To delete a pair, highlight the pair in the Correlated Pairs Specified area. This will enable the Delete Pair button. Click on this button and the pair will be removed from the list.

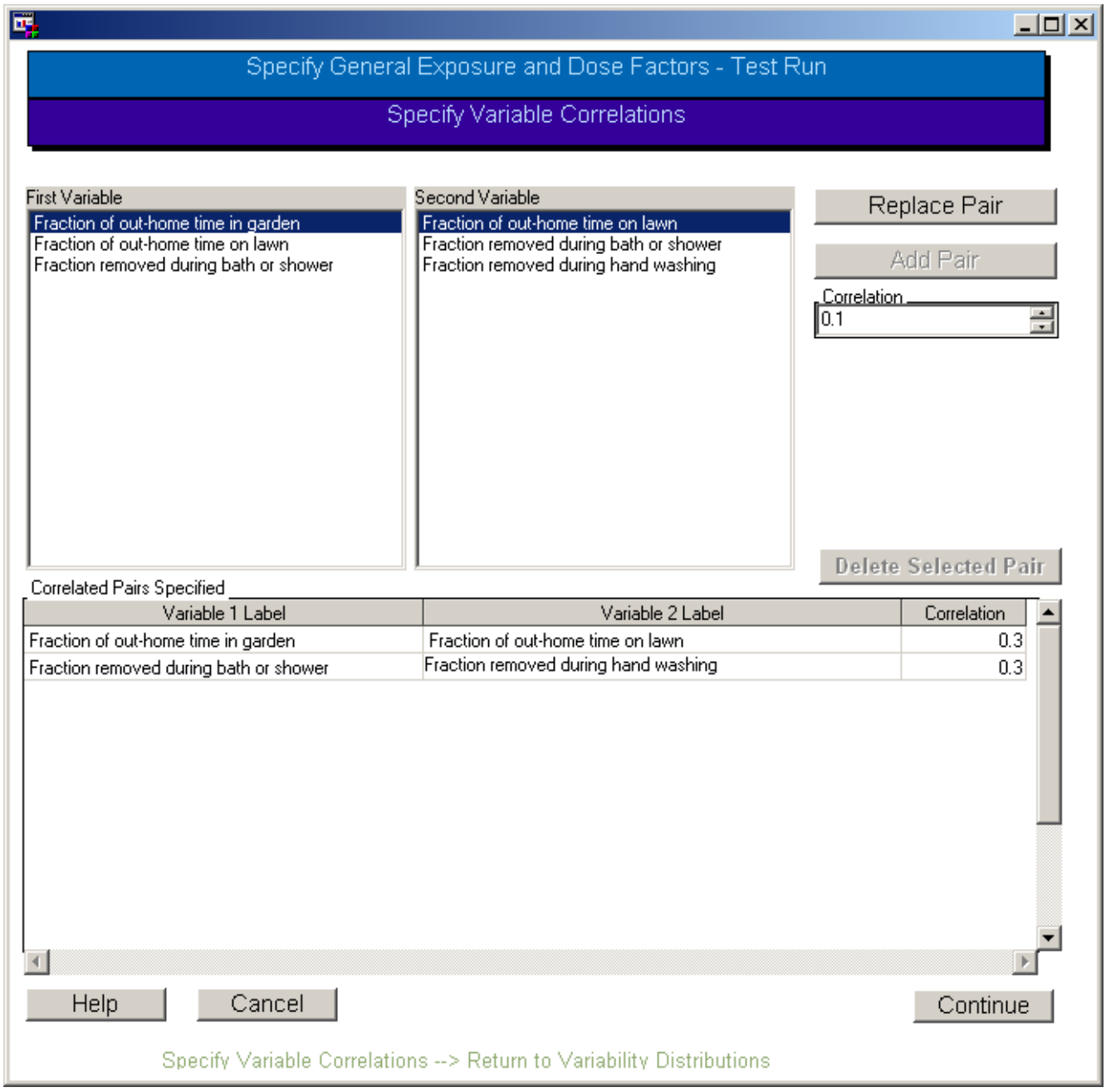


Figure 5.40. Specify Variable Correlations Screen.

Clicking on Continue saves the values defined and returns the user to the Variability Distributions screen. Once uncertainty is implemented, the user will be returned to the Uncertainty Distributions screen if doing an uncertainty run.

If no correlated pairs are chosen, then an error screen will be displayed (Figure 5.39), and correlation will be turned off in the simulation. Begin from the Variability Distributions screen to turn correlated inputs on once again.

5.10 Run Simulation

Only when all information has been specified will the Run Simulation button on the main menu (see Figure 5.2) be enabled. Clicking on it brings the user to the Run Simulation screen (Figure 5.41). The screen displays the current run name, the number of simulated profiles, the number of sensitivity or uncertainty repetitions (if any), the number of chemicals, and estimated run time. If 20 or fewer people are being simulated, then the user will have the option of turning on the diagnostic mode.

"Write Inputs to Excel" generates a file containing all of the user editable model inputs. The file is an XML file, but can be read by MS Excel 2003 or later. The file is placed in the install directory and is named using the run name and the standard Excel file extension (.xls).

"Check Input for Errors" forces two routines to run and check inputs. Comments and errors will be displayed to the log which will be made visible if is not already. These same checks are also carried out when the simulation is run.

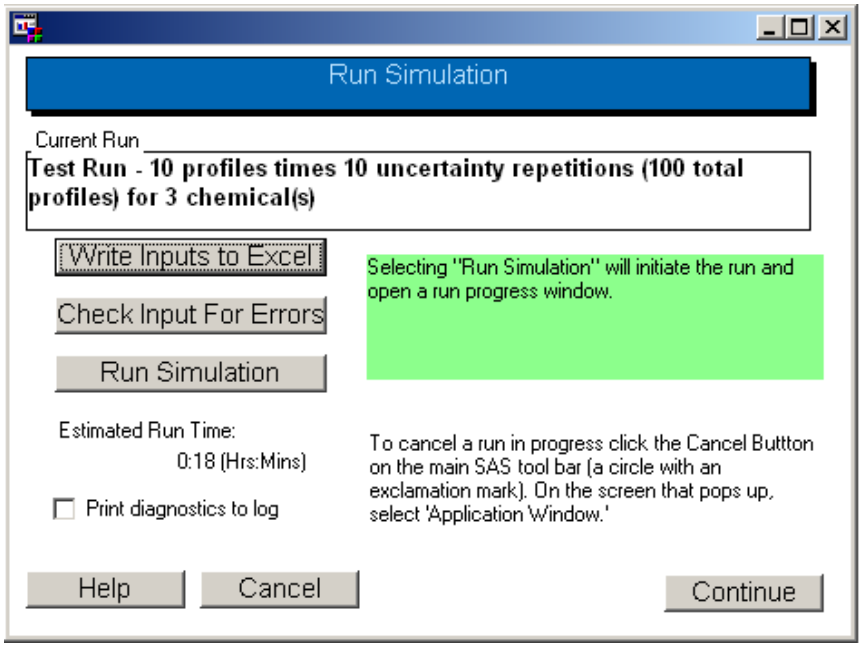


Figure 5.41. Run Simulation Screen for an Uncertainty Run.

Clicking on "Run Simulation" will begin the simulation. This will open the Run Progress Screen (Figure 5.42). This screen contains information about the progress of the run, including how

many profiles and chemicals have been completed, the estimated remaining time, and the average time per profile. For a sensitivity or variability run, the screen will also indicate which sensitivity or uncertainty repetition is currently being performed. In addition, informational messages will be displayed in the log (Figure 5.43). Among other items, the number of people completed and the number total are indicated as the run progresses. When the simulation is completed, the final timing information will be displayed in the log. Clicking the Continue button after run completion will return one to the main menu where View Results can be selected.

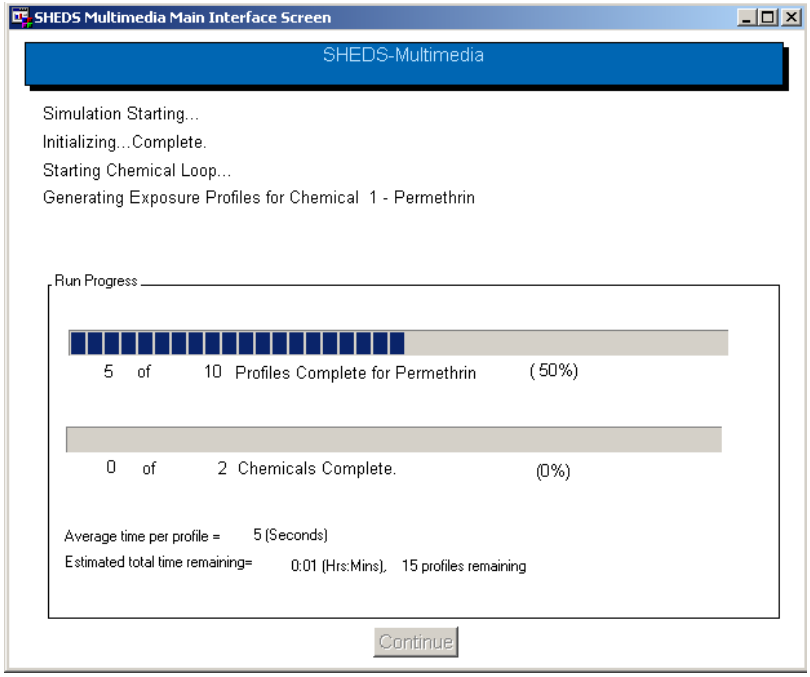


Figure 5.42. The Run Progress Screen for a Variability Run.

Typically you will want to open the log window before running a simulation. If the log window has been minimized, clicking the button along the bottom of the main SAS window will open it. This can be done after the run has started. If not open yet, the log window can be opened by selecting the View menu on the main SAS menu bar and then selecting Log. This must be done before the simulation has started.

The correlated pairs are checked for validity at the beginning of the run. If problems are found an error message will be printed in the log.

The diagnostic mode is only available for simulations with twenty or fewer people. Typically, a user will not want to run in diagnostic mode. If one is very familiar with the model it may be helpful in locating errors. Three things happen when the model is run in diagnostic mode.

1. SAS prints detailed notes to the log detailing how macros were compiled and data steps completed.

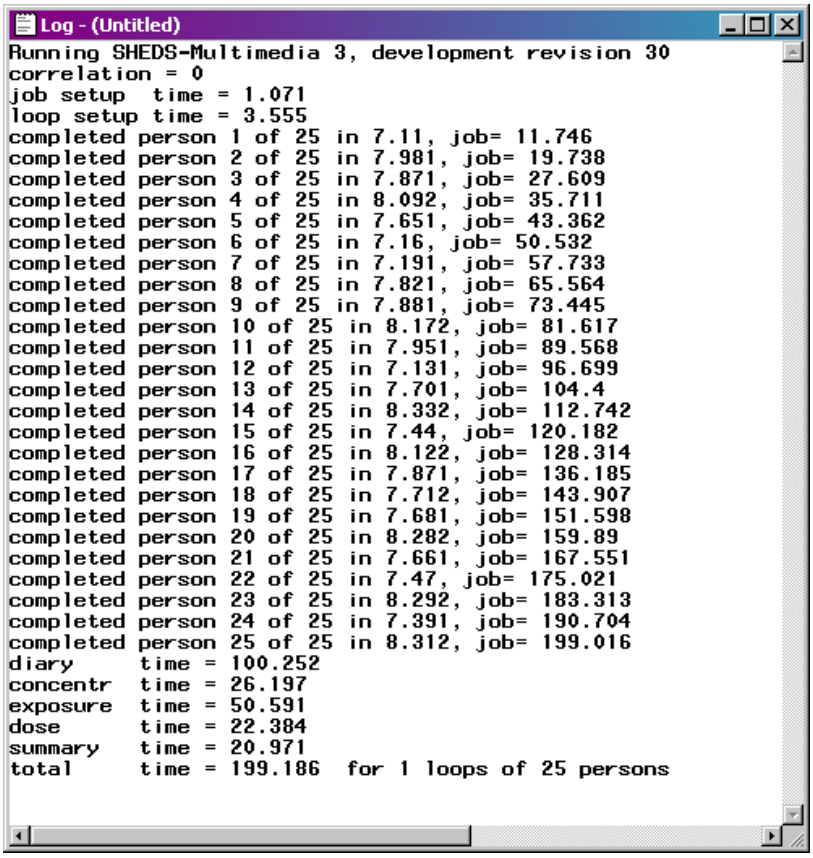


Figure 5.43. Log Screen after Running a Small Simulation.

2. Intermediate variables are saved on the datasets. This option is also available on the Simulation Information screen.
3. Event level datasets and variables are saved for each individual simulated.

Once started, the run can be cancelled by following the instructions on the Run Dialog.

5.11 View Results

Model results from previous or current SHEDS simulations can be viewed by selecting the View Results button on the main window. This button will become active once a simulation run has been made or after a previously run simulation is specified in the Run Name dialog. Pressing this button opens a dialog (Figure 5.44) allowing the user to select one of the following:

- View Results for the Population;
- View Results for an Individual;
- View Uncertainty Results;

- View Sensitivity Results;
- View Diary Pool Sizes.

Each of these buttons opens a new dialog.

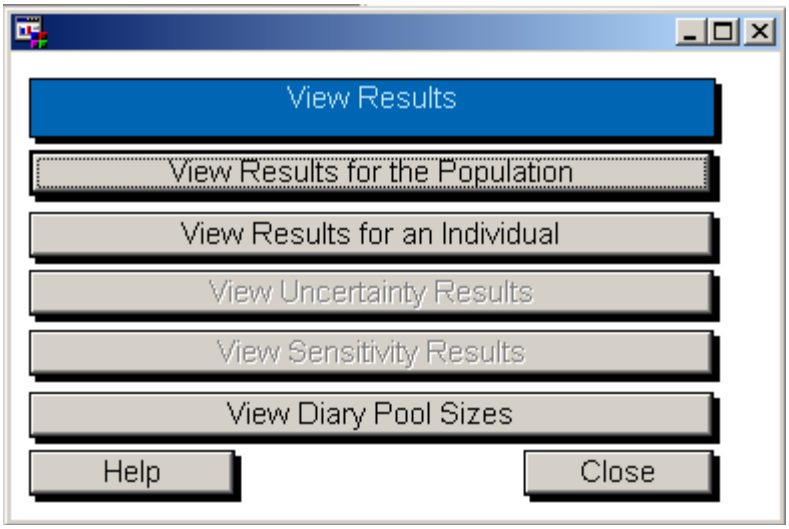


Figure 5.44. View Results Screen.

5.11.1 Additional Outputs and Files

A number of outputs cannot be viewed through the interface. For information on the log files, export files, and exporting files from SAS for analysis in other software, see Appendix A for more information.

5.11.2 View Results for the Population

The View Results for the Population window is used to generate graphical or tabular results for output variables for the population as a whole, or for subgroups of the population. The outputs will utilize the average daily values for the simulation just run or that specified most recently in the Run Names dialog. When considering the population, the output variables utilized are the daily values (of exposure, dose, etc.) for each person, averaged over the simulation period. The outputs generated examine the variability of these personal mean daily values over the population. In addition, the personal daily maximums for each person for each variable can also be viewed.

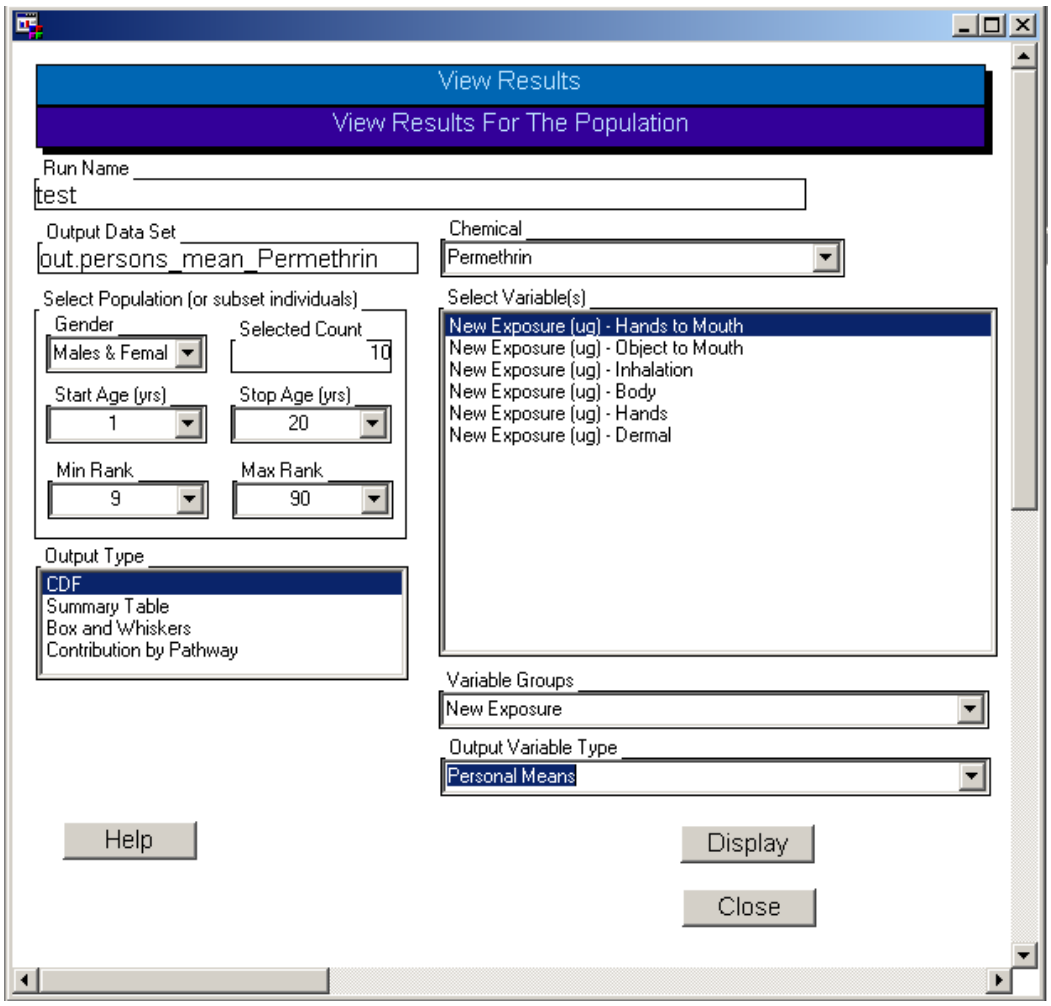


Figure 5.45. View Results for the Population Screen.

In general the user will want to work from the top down, selecting the output units and thus the output dataset of interest, then the sub-population of interest, output type, and specific variables desired.

The Run Name box shows the name of the current run, while the Output Data Set supplies the name of the corresponding SAS dataset that will be used to generate the results.

The Output Units menu is used to indicate the units for the output data, either Milligrams per Kilogram body weight or Micrograms. The appropriate output dataset will be displayed in the Output Data Set box.

The menus in the Select Population box (Gender, Start Age, Stop Age, Min Rank, and Max Rank) can be used to select a subgroup of the run population for analysis. Subsetting is based on the fact that each simulated individual is assigned a specific age, gender and bin rank. The entire simulated population is divided into 100 bins labeled 0 to 99; as nearly as possible, the bins contain the same number of people. (If the simulated population is less than 100, some of the bins will be empty and will not appear in the pull down menu.) The bins are ranked based on the total chemical absorption over the entire simulation period. The user may subset the population by restricting the age range, gender, bin rank, or any combination of these. For example, the user may choose to examine only the women or only the children. The pull down menus only display genders, ages, and ranks that exist in the output dataset. The final selections and count of individuals will appear on any resulting tables and graphics generated. The Selected Count field updates after each user selection to display the final number of people in the sub-group.

The Output Type list box includes the analyses that may be performed. The user selects one option from this list at a time. The options for results analyses in SHEDS-Residential version 4 are the following:

- Summary Table;
- CDF (Cumulative Distribution Function);
- Box and Whiskers; and
- Contribution by Pathway.

The Chemical list box lets the user select the chemical for which to view any chemical-specific results (like exposures and doses). All chemicals in the simulation will be available for viewing. In addition, for cumulative runs, the variable "Cumulative" will also be available in the chemical list. Selecting this variable will allow the user to view the results that result from combining the results for all the chemicals in the run. Any non-chemical specific variables (such as Ventilation) will display the same results for any selection from the chemical list box.

For uncertainty and sensitivity runs, the summary sensitivity and uncertainty results are viewed on screens specific to these types of runs (see following sections). However, for each of these types the user can also view the variability results from each variability repetition. For these types of runs, there will be an additional list box on the View Results for the Population screen labeled "Uncertainty Repetition" or "Sensitivity Repetition". This box will contain a list of the available repetitions. The user can then select any of the repetitions to view.

The Variable Groups list box allows the user to select a subgroup of the variables to view. When the user selects a group, the available variables will appear in the Select Variables selection box. The available variable groups are:

- New exposure;
- New exposure normalized to body mass;

- New handler exposure;
- Running exposure;
- New dose;
- New dose normalized to body mass;
- Ventilation;
- Chemical and metabolite entering blood;
- Eliminated chemical; and
- Margin of exposure.

See the Technical Manual for the definitions of these terms.

The Output Variable Type list box lets the user select either:

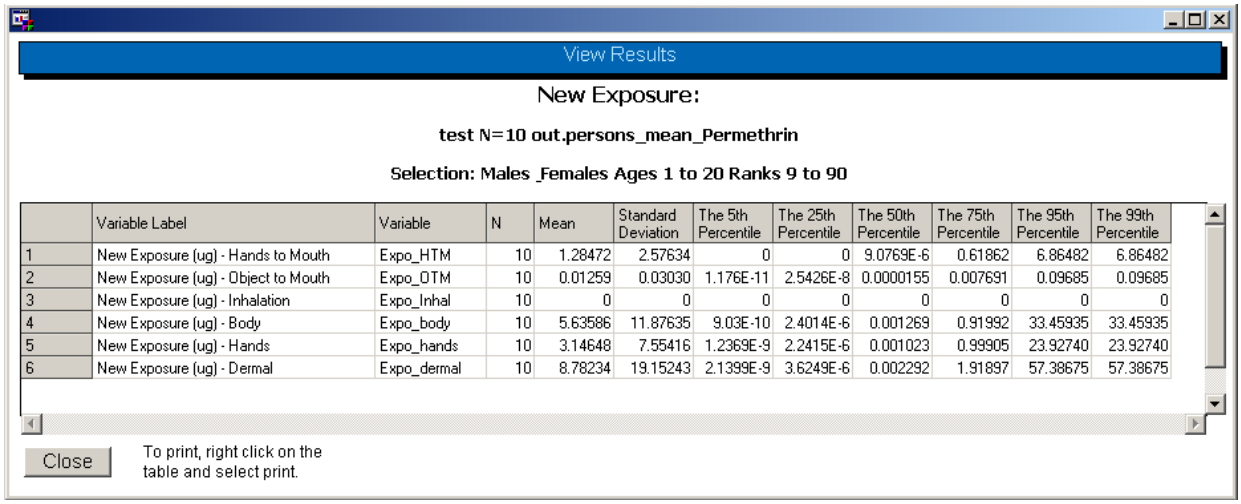
- Personal Means; or
- Personal Maximums.

Pressing the Display button then performs the analysis and displays the results in a new window. That window must be closed to return to this dialog to define new outputs.

The Variable Groups and Select Variables menus are used to select the model output variables to analyze. The Variable Groups menu is used to pick a general category of model variables (such as dose, exposure, or loading variables). Selecting this variable group will update the Select Variables menu to include all corresponding model variables. For example, in Figure 5.45 the Variable Group selected is New Exposure, so the Select Variables menu has been updated to include all the corresponding exposure variables. The user then selects one or more variables from this list to analyze. Clicking on display generates the output. Specific details of each of the Output Types are covered next.

5.11.2.1 Summary Table

Selecting this option yields a summary statistics table for the selected variable(s) and specified model simulation, including sample size, mean, standard deviation, median, 5^{th},25^{tt}, 75^{th}, 95^{th}, and 99^{th} percentiles. An example is shown in Figure 5.46. If multiple variables are analyzed, the results are displayed on individual rows of the table; the variable name and description (label) are included on each row. Again, note that the subpopulation that is being examined is printed in the table window – in this hypothetical example the user is examining males and females between the ages of 1 and 20 years.



	Variable Label	Variable	N	Mean	Standard Deviation	The 5th Percentile	The 25th Percentile	The 50th Percentile	The 75th Percentile	The 95th Percentile	The 99th Percentile
1	New Exposure (ug) - Hands to Mouth	Expo_HTM	10	1.28472	2.57634	0	0	9.0769E-6	0.61862	6.86482	6.86482
2	New Exposure (ug) - Object to Mouth	Expo_OTM	10	0.01259	0.03030	1.176E-11	2.5426E-8	0.0000155	0.007691	0.09685	0.09685
3	New Exposure (ug) - Inhalation	Expo_Inhal	10	0	0	0	0	0	0	0	0
4	New Exposure (ug) - Body	Expo_body	10	5.63586	11.87635	9.03E-10	2.4014E-6	0.001269	0.91992	33.45935	33.45935
5	New Exposure (ug) - Hands	Expo_hands	10	3.14648	7.55416	1.2369E-9	2.2415E-6	0.001023	0.99905	23.92740	23.92740
6	New Exposure (ug) - Dermal	Expo_dermal	10	8.78234	19.15243	2.1399E-9	3.6249E-6	0.002292	1.91897	57.38675	57.38675

Figure 5.46. Example Summary Table for a Population.

5.11.2.2 CDF

This option yields a cumulative distribution function (CDF) plot for the selected variable(s) and specified model simulation. The plot illustrates how the percentiles of the selected variable(s) behave as a function of the variable value. Each selected variable will appear as a separate line on the plot; a legend appears at the bottom of the plot to identify each variable. An example is shown in Figure 5.47. In the example, the CDFs for six new exposure variables are plotted (only three can be seen in this particular case, since all the percentiles for the others were zero in this simulation.) The plot can be printed by clicking on the Print button. The default printer will be used and the plot will be formatted for default SAS printer.

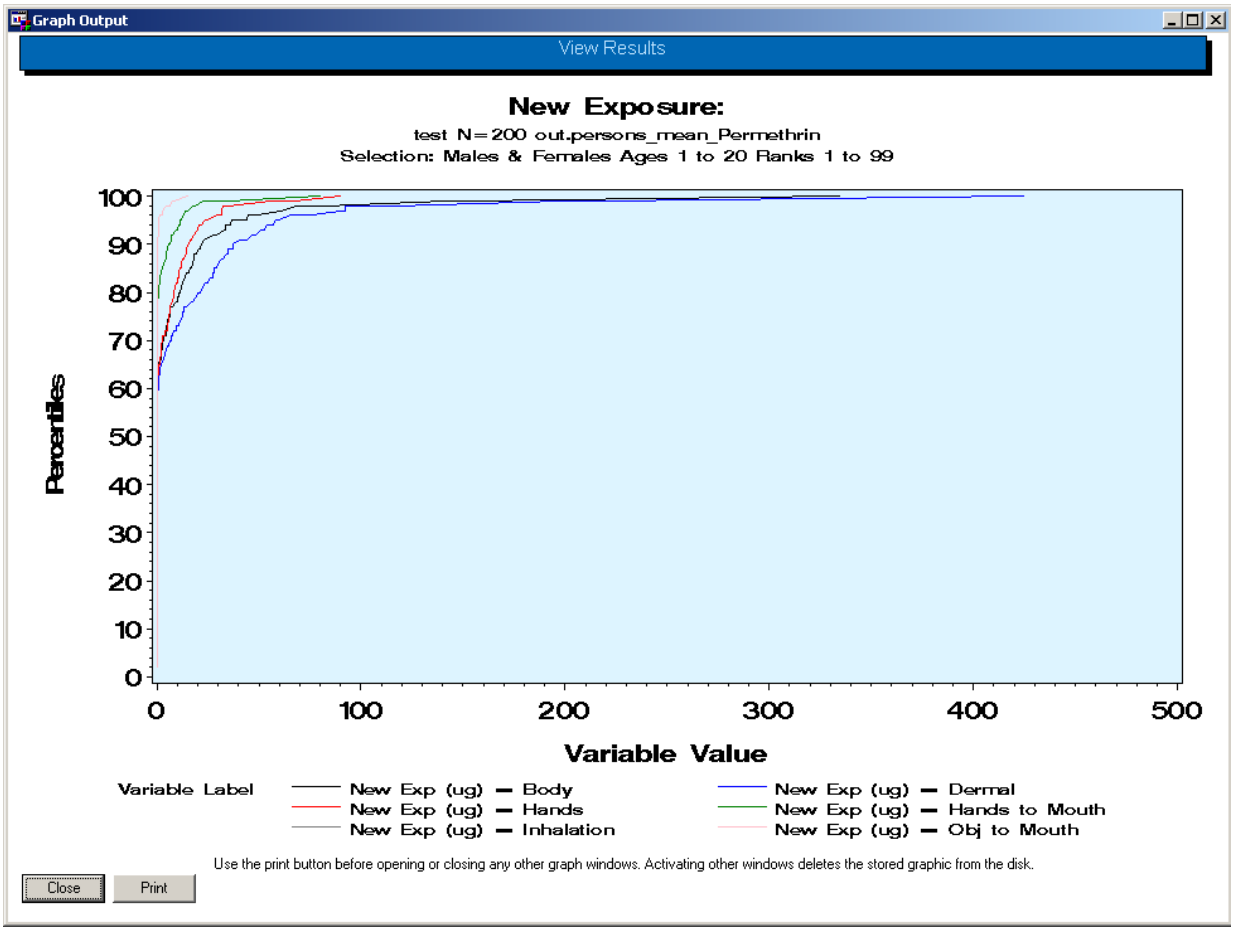


Figure 5.47. Example CDF for a Population.

5.11.2.3 Box and Whiskers

Selecting the Box and Whiskers option yields a box and whiskers plot for the selected variable(s) for the current simulation for the defined population subgroup. Multiple variables are shown on a single plot. An example for seven absorption variables is given in Figure 5.48. Unlike other plots, the Box and Whiskers plots use the variable names rather than the variable labels. The longer labels will overwrite one another or be suppressed by SAS. The boxes, whiskers, and other symbols on the plot are interpreted as follows:

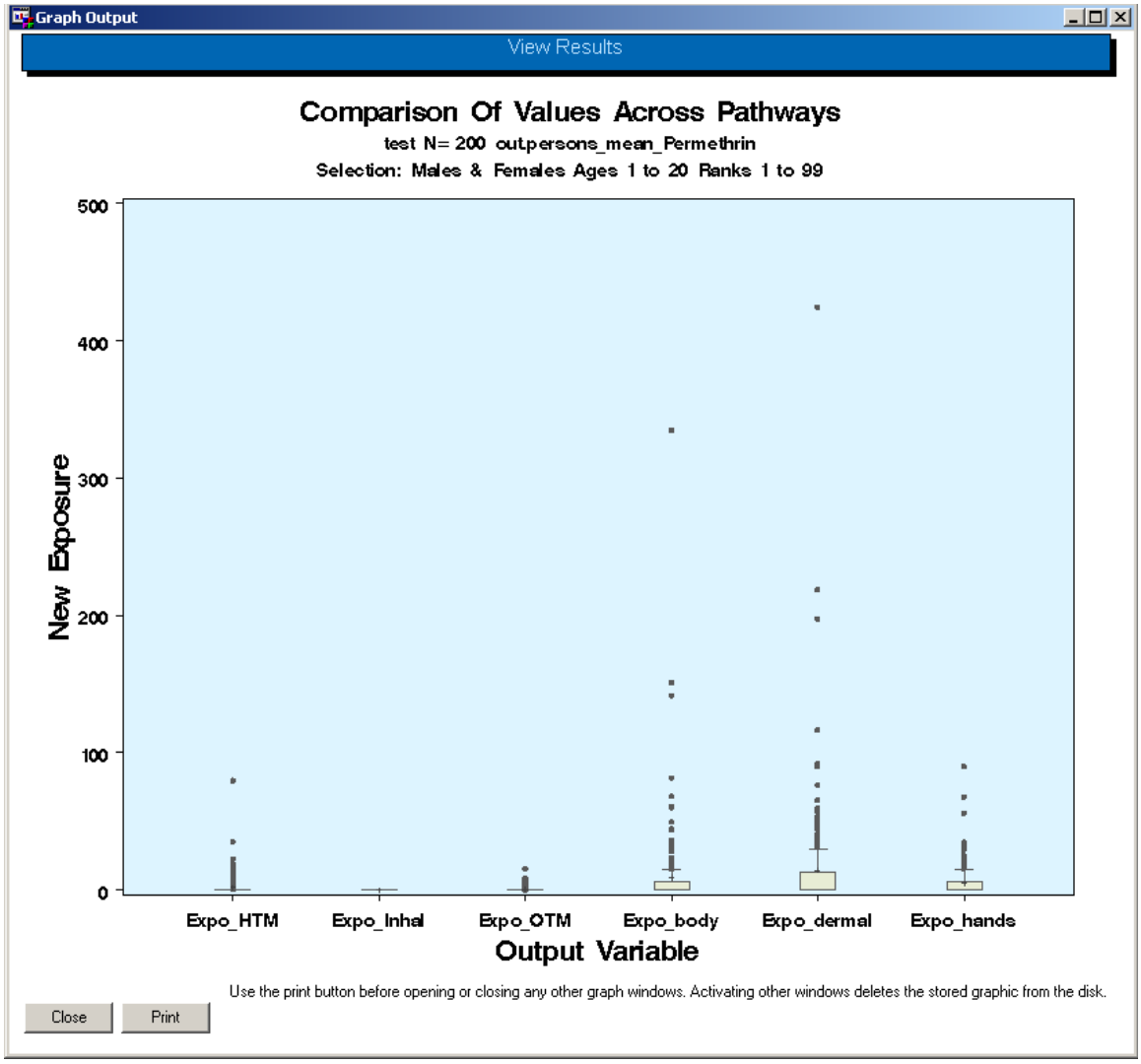


Figure 5.48. Example Population Box and Whiskers Plot.

- The midlines of the boxes are equal to the median.
- The plus (+) symbol inside the boxes is equal to the mean.
- The upper edge of the box is the 75th percentile of the population, while the lower edge is the 25th percentile. Thus, these edges define the width of the interquartile range (IQR).
- The whiskers define the maximum or minimum observations that fall within 1.5 times the IQR, measured from the quartile value (i.e., the 75th or 25th percentile).

- The square symbols indicate data points outside of the range defined by 1.5 times the IQR.

5.11.2.4 Contribution by Pathway

The Contribution by Pathway option is different from the other options in the Output Type menu. It does not require (or allow) selection of individual model variables. Only a selection from the Variable Group menu is required: New Exposure, New Exposure Normalized to Body Mass, New Handler Exposure, Running Exposure, New Dose, or New Dose Normalized to Body Mass. Clicking on Display yields a pie chart showing percent contribution to one of these summary variables (based on population or population subgroup means or maxes) for the following pathways:

- Dermal;
- Inhalation;
- Ingestion;
- Hand-to-Mouth; and
- Object-to-Mouth.

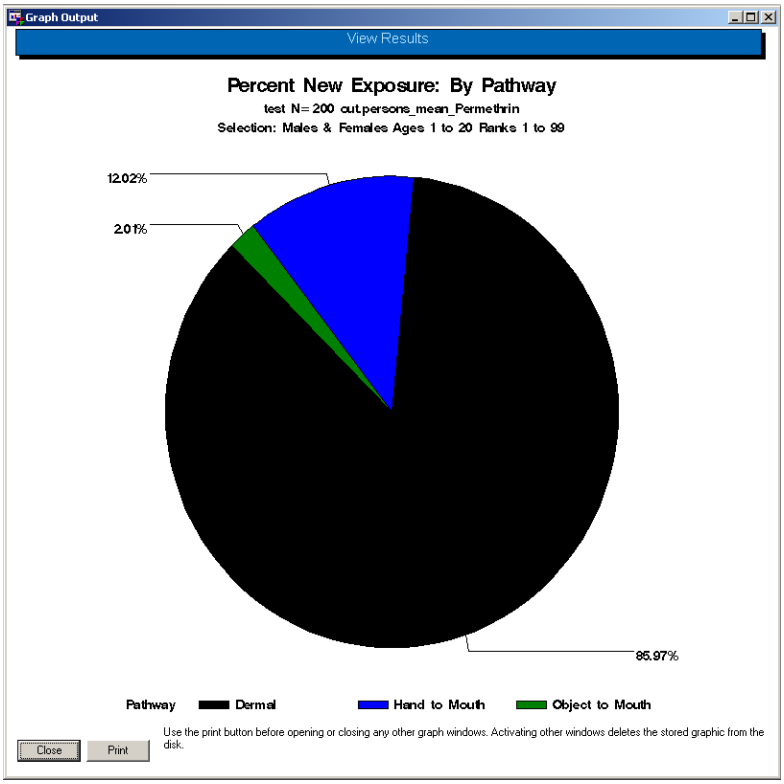


Figure 5.49. Example Pie Chart Showing the Contribution by Pathway for a Population.

5.11.3 View Results for an Individual

The second results window accessible from View Results is the View Results for Individual. Selecting this button brings up the window for performing analysis of the results for a single individual within a simulation run. Many of these options are similar to those for View Results for Population. When considering an individual, the output variables of interest are the daily values for the selected individual. A specific simulated individual must be selected. Additionally, the analysis may be limited to a specific time period. As on the population results screen, it is best to work from the top down on the left side of the screen, and then choose the Variable Group and specific variables of interest. All resulting outputs will contain a second title giving the basic individual statistics and dates considered in the analysis.

The View Results for an Individual dialog is shown in Figure 5.50. The Run Name box shows the name of the current run, while the Output Data Set supplies the name of the corresponding SAS dataset that will be used as the basis of the results. The output dataset is dependent on the units chosen. As in the Results for Population window, one can select genders, an age range, and a rank range in the Select Population box. In this case, the Select Individuals list box is populated only with individuals meeting these criteria. The individual list box provides minimal information on each individual: the identifier used in the simulation, the gender (shown as 'M' or 'F'), age, and the individual's rank or percentile of total absorption. The user clicks on an individual to select and then analyze data from that individual.

In addition to selecting an individual, the user may also select a particular range of dates to analyze from the Dates of Interest menu. The Start Date and Stop Date may be selected from the corresponding menus, which are populated with all the dates covered by the current simulation.

The output options for viewing variability results for an individual are listed in the Output Type list box. These include:

- Time-Series;
- CDF (Cumulative Distribution Function);
- Box and Whiskers;
- Contribution by Pathway;
- Summary Table; and
- Detailed Table.

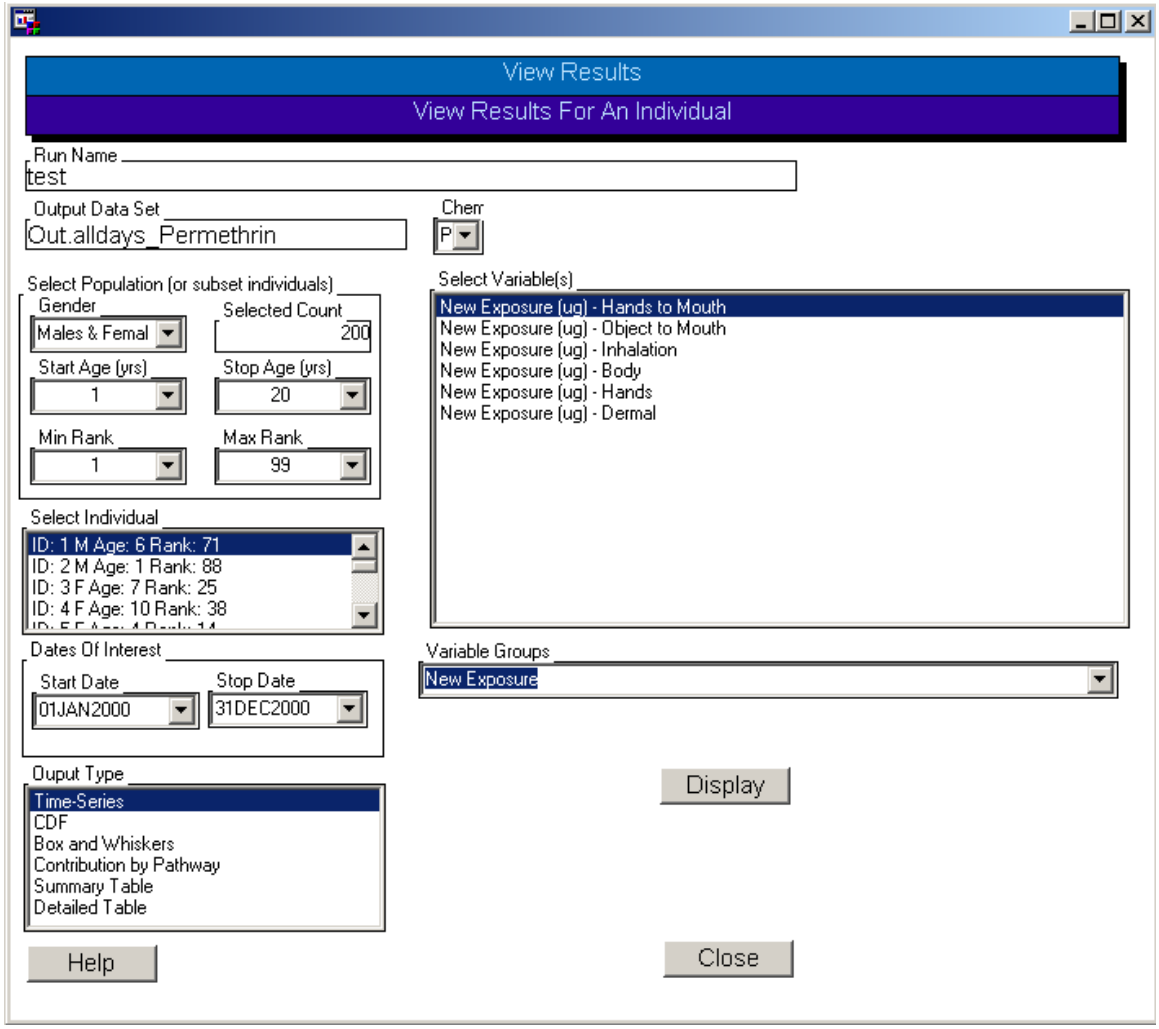


Figure 5.50. View Results for an Individual Screen.

The user also must select the chemical for which to view results, and a Variable Group. These list boxes behave the same as on the View Results for Population Screen (Section 5.11.2).

The user may also view individual results for uncertainty and sensitivity runs; however, in this case, only the individuals simulated in the very last sensitivity or uncertainty repetition are available. Due to space limitations, SHEDS does not retain daily-level information for every repetition (only the most recent). It should be noted that while all repetitions are valid variability runs, one should use caution when viewing results from a percentile scaling run, because in this type of run certain variables (most sensitivity input variables) may be being held at their median values in the last sensitivity repetition.

As in the View Results by Population dialog, the output units may be selected as either Microgram or Milligrams per Kilogram from the Output Units menu, and the Variable Groups and Select Variables menus are used to select the model output variables to analyze. As before, multiple variables may be selected for analysis. The appropriate analysis variables will automatically be chosen for Contribution By Pathway. All variables will automatically be used for the detailed table. Each of the output types are described next.

5.11.3.1 Time-Series

Selecting the Time-Series button produces a time-dependent plot of the selected variable(s). Each data value on the plot is the value for a single day in the simulation. Multiple variables will be plotted as multiple curves on the same time-series plot; the legend that appears at the bottom of the plot identifies which variable is associated with each plotted curve. Time-Series simulations are useful for observing the behavior of doses and exposures in the days following a pesticide application. An example showing six exposure variables (some of them essentially equal to 0) is given in Figure 5.51.

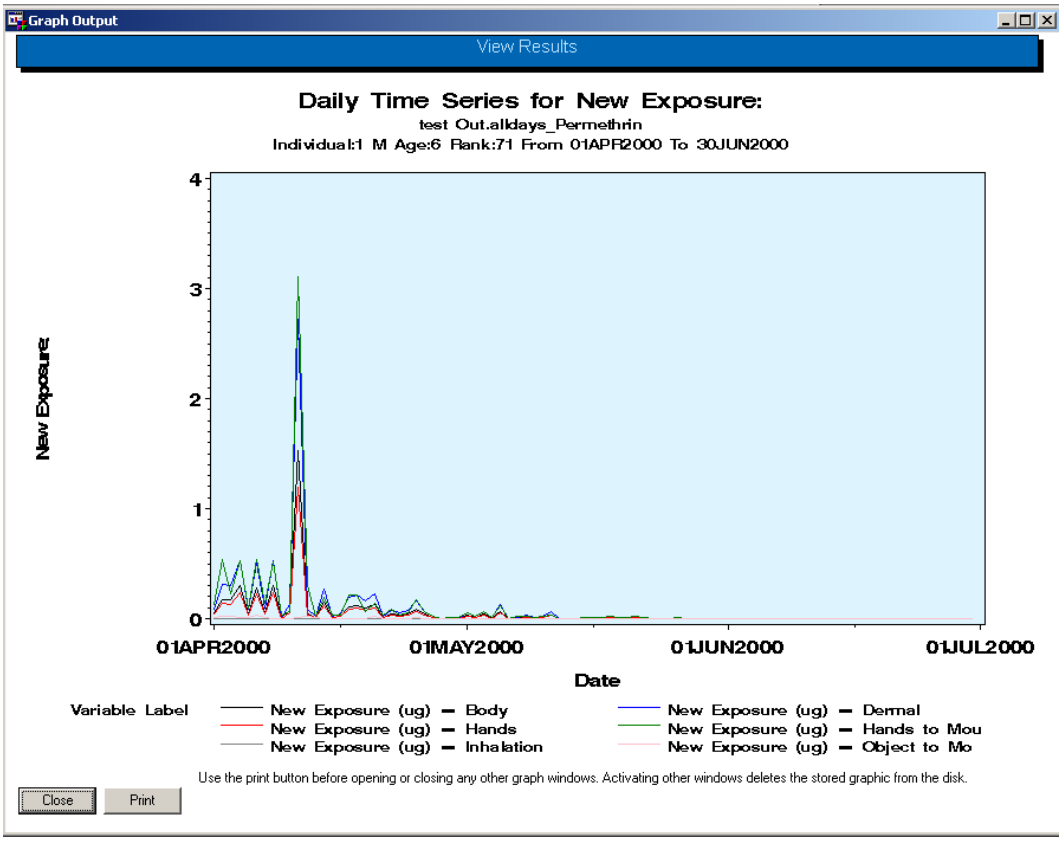


Figure 5.51. Example Time-Series for an Individual.

5.11.3.2 CDF

The CDF option for an individual is similar to that for the population (See Figure 5.47). The option yields a cumulative distribution function plot for the daily values of the selected variable(s) for the specified individual. Each selected variable will appear as a separate line on the plot; a legend appears at the bottom of the plot to identify each variable. An example of a CDF for an individual for new dermal exposure for a year-long simulation is given in Figure 5.52.

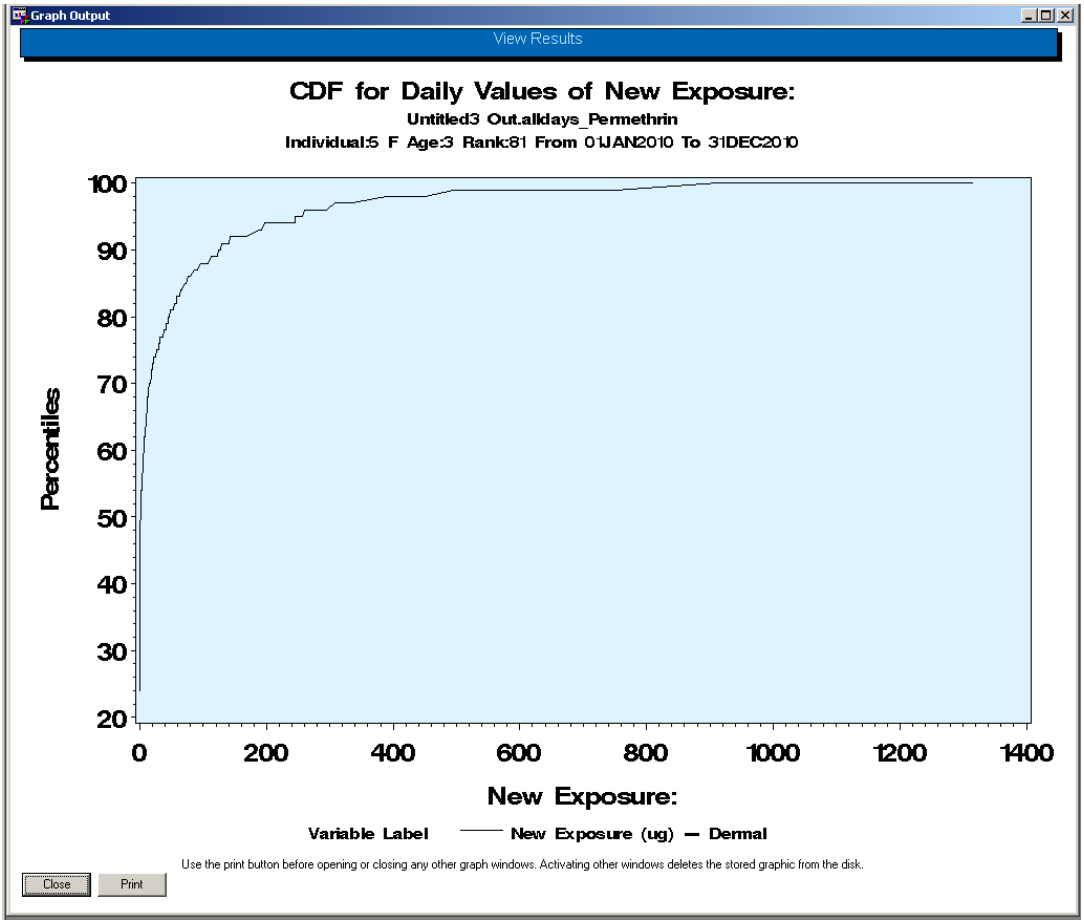


Figure 5.52. Example CDF for an Individual.

5.11.3.3 Box and Whiskers

The Box and Whiskers option for an individual is similar to that for the population (see Figure 5.48 on page 80 and the previous discussion), with the exception that the plot is generated by examining the daily variable values for a single person rather than the mean daily values for the population. Selecting Box and Whiskers and clicking on Display will yield a plot for the selected variable(s) for the current simulation, selected person, and selected dates. Multiple variables are shown on a single plot. An example box and whiskers plot for an individual's daily values of several new dose variables for a year-long simulation is shown in Figure 5.53.

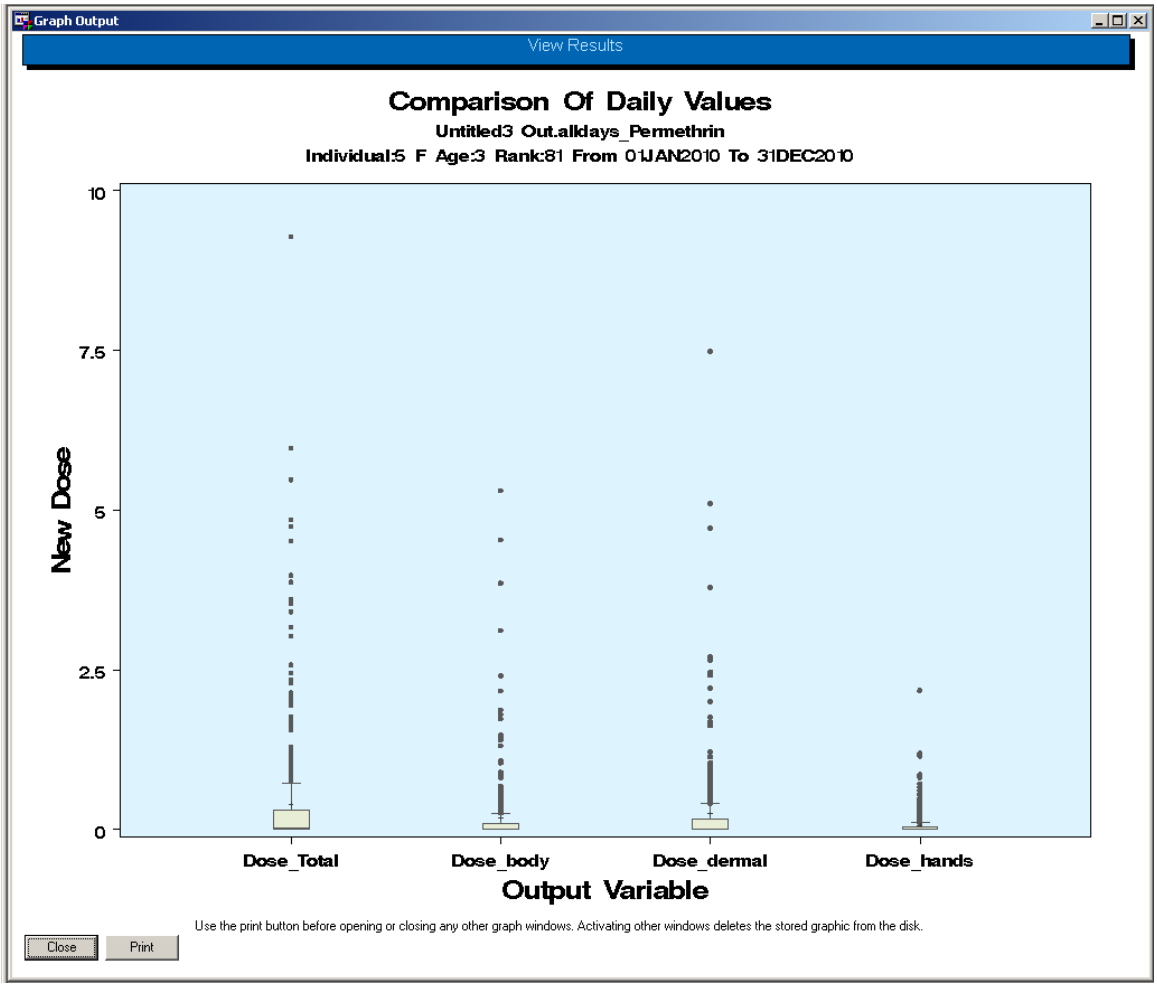


Figure 5.53. Example Box and Whiskers Plot for an Individual.

5.11.3.4 Contribution by Pathway

The interpretation of the Contribution by Pathway option for an individual is identical to that for the population. As before, this option does not require or permit selection of individual model variables; only the Variable Group needs to be specified-- New Exposure, New Exposure Normalized to Body Mass, New Handler Exposure, Running Exposure, New Dose, or New Dose Normalized to Body Mass. (The Select Variables menu will be inactive if Contribution by Pathway is selected). Selecting Display then yields a pie chart showing percent contribution to one of these summary variables by pathway.

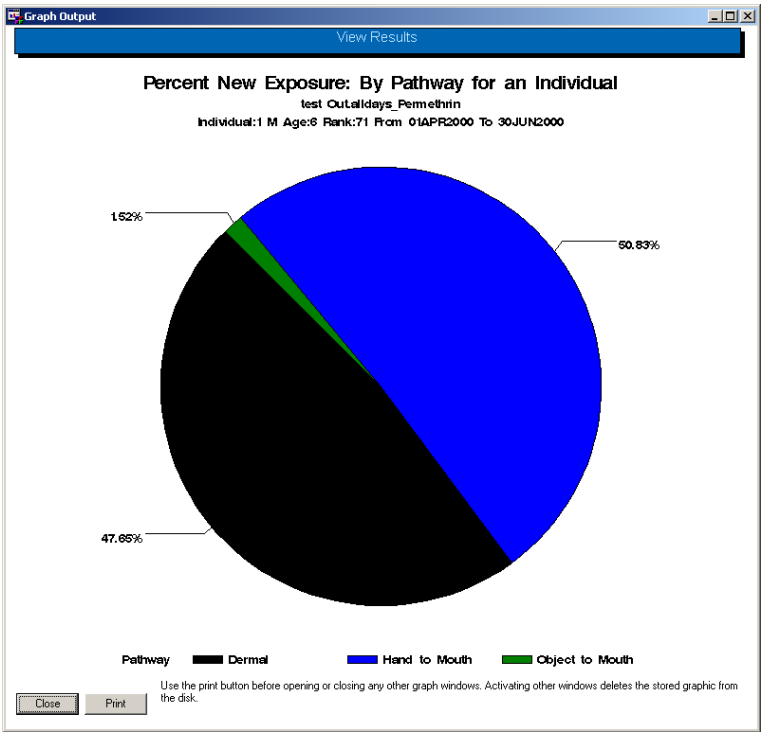


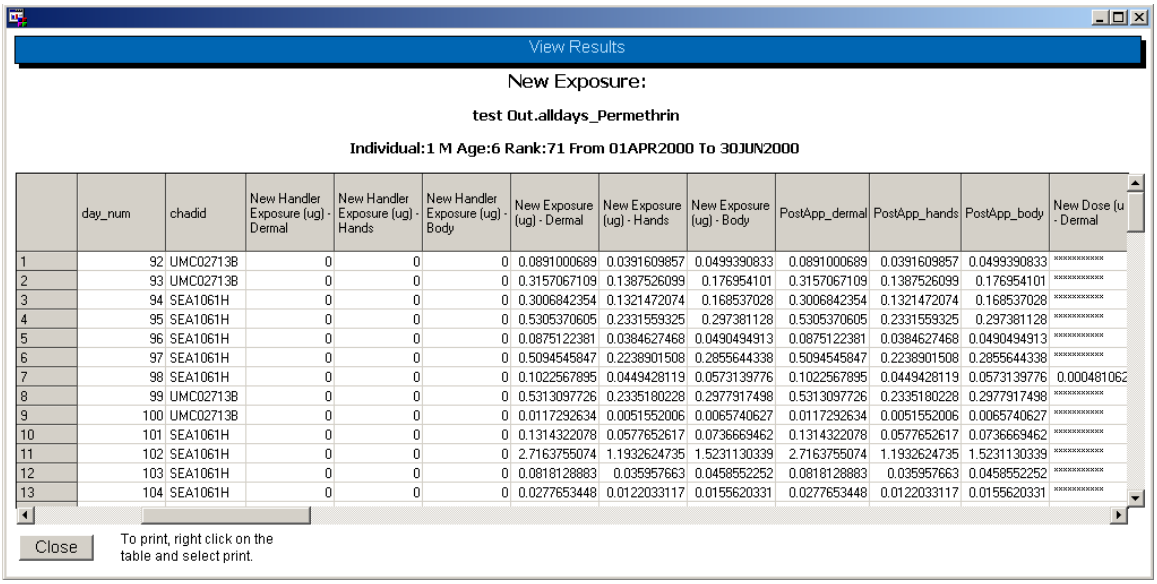
Figure 5.54. Example Pie Chart Showing the contribution by pathway for an individual.

5.11.3.5 Summary Table

If Summary Table is selected, clicking on Display will open a new window containing the percentiles of the selected variable(s), with each variable appearing on its own row in the table. Specifically, the table contains the sample size, mean, standard deviation, median (p50), 5th percentile (p05), 25th percentile (p25), 75th percentile (p75), 95th percentile (p95), and 99th percentile (p99). The age and gender of the individual being examined appears in the descriptive heading. The resulting table looks very similar to the summary table for the population (see Figure 5.46), with the exception that the statistics represent the variation in the variables across days for a single person (rather than the variation in the averaged daily values across persons).

5.11.3.6 Detailed Table

Selecting the Detailed Table option opens a new window and displays a table that contains detailed information for all daily average variables generated by the model (Figure 5.55). It is not required or permitted to select a variable group or specific variables. The detailed table contains one row for each of the days being analyzed. The table contains the year, month, and day, the number of diary events for the day, and the values for each model variable related to the Variable Group. All variables will not fit on the screen at once. The scroll bar at the bottom of the window can be used to view the variables that appear to the right.



	day_num	chadid	New Handler Exposure (ug) - Dermal	New Handler Exposure (ug) - Hands	New Handler Exposure (ug) - Body	New Exposure (ug) - Dermal	New Exposure (ug) - Hands	New Exposure (ug) - Body	PostApp_dermal	PostApp_hands	PostApp_body	New Dose (u - Dermal
1	92	UMC02713B	0	0	0	0.0891000689	0.0391609857	0.0499390833	0.0891000689	0.0391609857	0.0499390833	**********
2	93	UMC02713B	0	0	0	0.3157067109	0.1387526099	0.176954101	0.3157067109	0.1387526099	0.176954101	**********
3	94	SEA1061H	0	0	0	0.3006842354	0.1321472074	0.168537028	0.3006842354	0.1321472074	0.168537028	**********
4	95	SEA1061H	0	0	0	0.5305370605	0.2331559325	0.297381128	0.5305370605	0.2331559325	0.297381128	**********
5	96	SEA1061H	0	0	0	0.0875122381	0.0384627468	0.0490494913	0.0875122381	0.0384627468	0.0490494913	**********
6	97	SEA1061H	0	0	0	0.5094545847	0.2238901508	0.2855644338	0.5094545847	0.2238901508	0.2855644338	**********
7	98	SEA1061H	0	0	0	0.1022567895	0.0449428119	0.0573139776	0.1022567895	0.0449428119	0.0573139776	0.000481062
8	99	UMC02713B	0	0	0	0.5313097726	0.2335180228	0.2977917498	0.5313097726	0.2335180228	0.2977917498	**********
9	100	UMC02713B	0	0	0	0.0117292634	0.0051552006	0.0065740627	0.0117292634	0.0051552006	0.0065740627	**********
10	101	SEA1061H	0	0	0	0.1314322078	0.0577652617	0.0736669462	0.1314322078	0.0577652617	0.0736669462	**********
11	102	SEA1061H	0	0	0	2.7163755074	1.1932624735	1.5231130339	2.7163755074	1.1932624735	1.5231130339	**********
12	103	SEA1061H	0	0	0	0.0818128883	0.035957663	0.0458552252	0.0818128883	0.035957663	0.0458552252	**********
13	104	SEA1061H	0	0	0	0.0277653448	0.0122033117	0.0155620331	0.0277653448	0.0122033117	0.0155620331	**********

Figure 5.55. Example Detailed Table for an Individual.

5.11.4 View Uncertainty Results

Selecting the View Uncertainty Results button from the View Results screen will open the window shown in Figure 5.56. This window allows the user to view several types of plots that summarize the uncertainty of the model as estimated from the uncertainty repetitions that were performed (i.e. the uncertainty that results from any uncertainty clouds that were defined for model variables using the "Uncertainty" type distribution.)

The variable group list is the same as on the other results screens. However, in the case of uncertainty runs, only a single variable can be selected at a time.

There are two types of output summary plots that are available for uncertainty runs:

- **Plot the 5th, 50th, and 95th percentile from each uncertainty repetition**. In this type of plot, the persons in each repetition with the 5th, 50th, and 95th population percentile average values for the variable are identified and these percentile values are retained and plotted as a CDF. An example of this type of plot is shown in Figure 5.57. In this example, five uncertainty repetitions were performed. A CDF is plotted of the population 5th, 50th, and 95th percentiles of total dose from each of these runs (and thus each CDF on the plot has 5 points). In this example, all the values of the 5th percentiles were 0, as were a number of the medians.

- **Plot the CDFs of repetitions whose medians are at the 5th, 50th, and 95th percentiles.** In this type of plot, three repetitions are identified: those whose population medians are at the 5th, 50th, and 95th percentile of all the repetition medians. An example of this type of plot is shown in Figure 5.58. In this example, total new dose was examined for an uncertainty run of 5 repetitions of 25 profiles each. Three repetitions were identified: that with a median with the 5th percentile of all medians. In this case, since only 5 repetitions were performed, the 5th percentile corresponded to the repetition with the lowest median. The 50th percentile corresponded to the repetition with the 3rd highest median out of the 5 run, and the 95th percentile corresponded to the repetition having the highest median. Then the population CDFs for total new dose are plotted for those three repetitions; note that each CDF has 25 points because 25 profiles were run. Note that this run is only for example purposes; many more profiles and repetitions would be needed to develop real, useful uncertainty results.

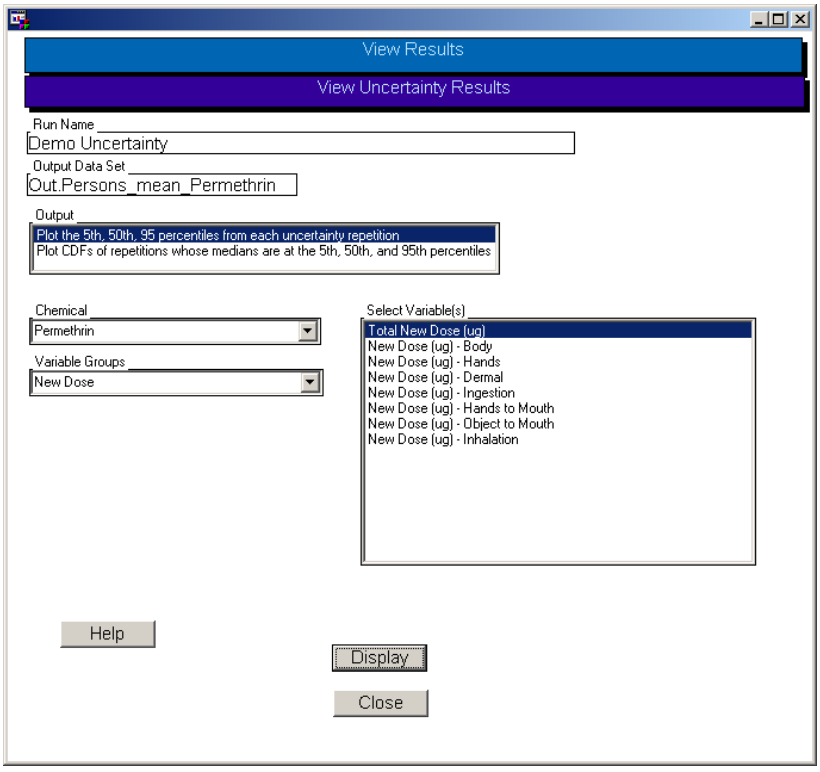


Figure 5.56. View Uncertainty Results Screen.

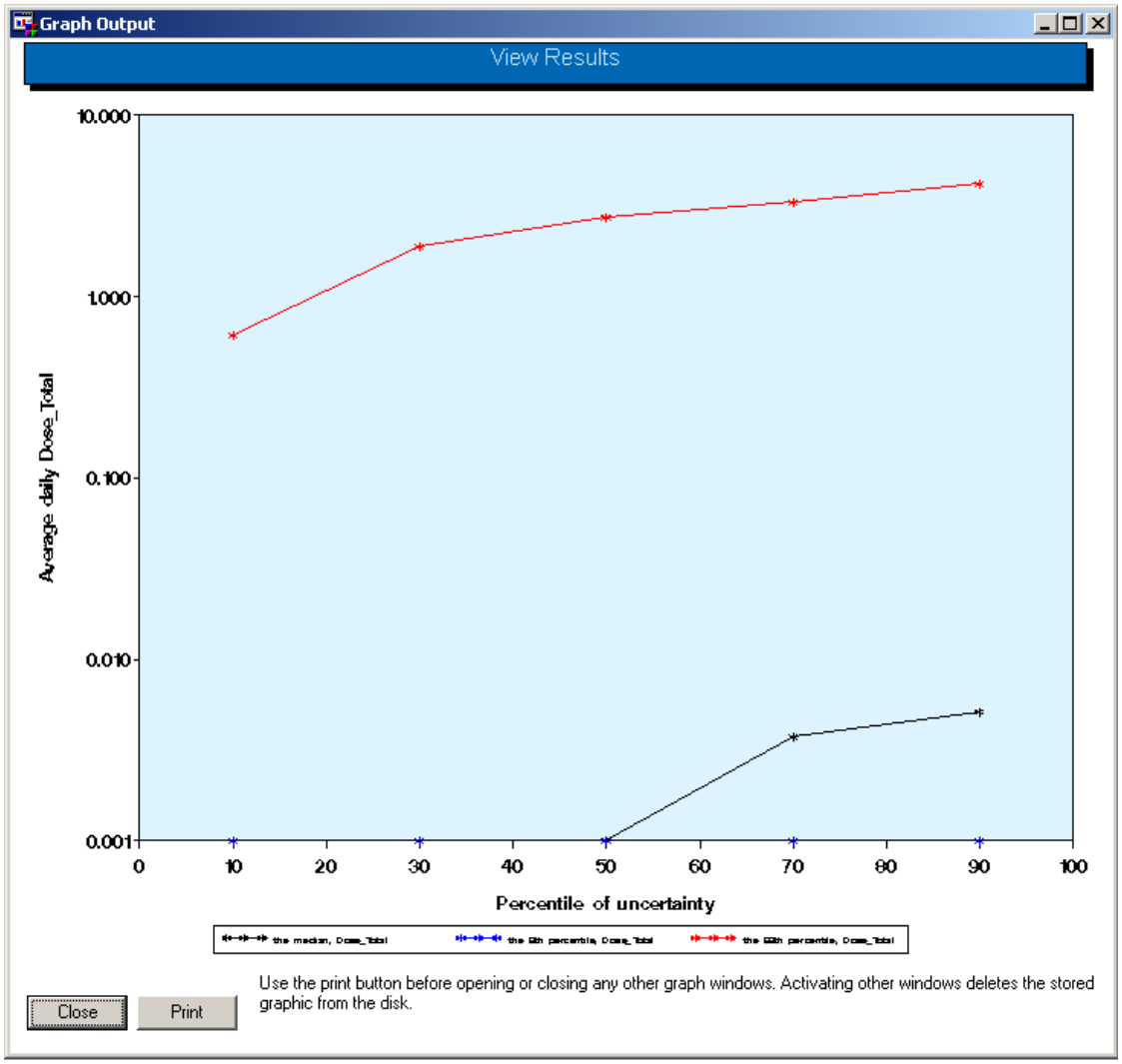


Figure 5.57. Plotting the 5th, 50th, and 95th Percentiles of Each Uncertainty Repetition.

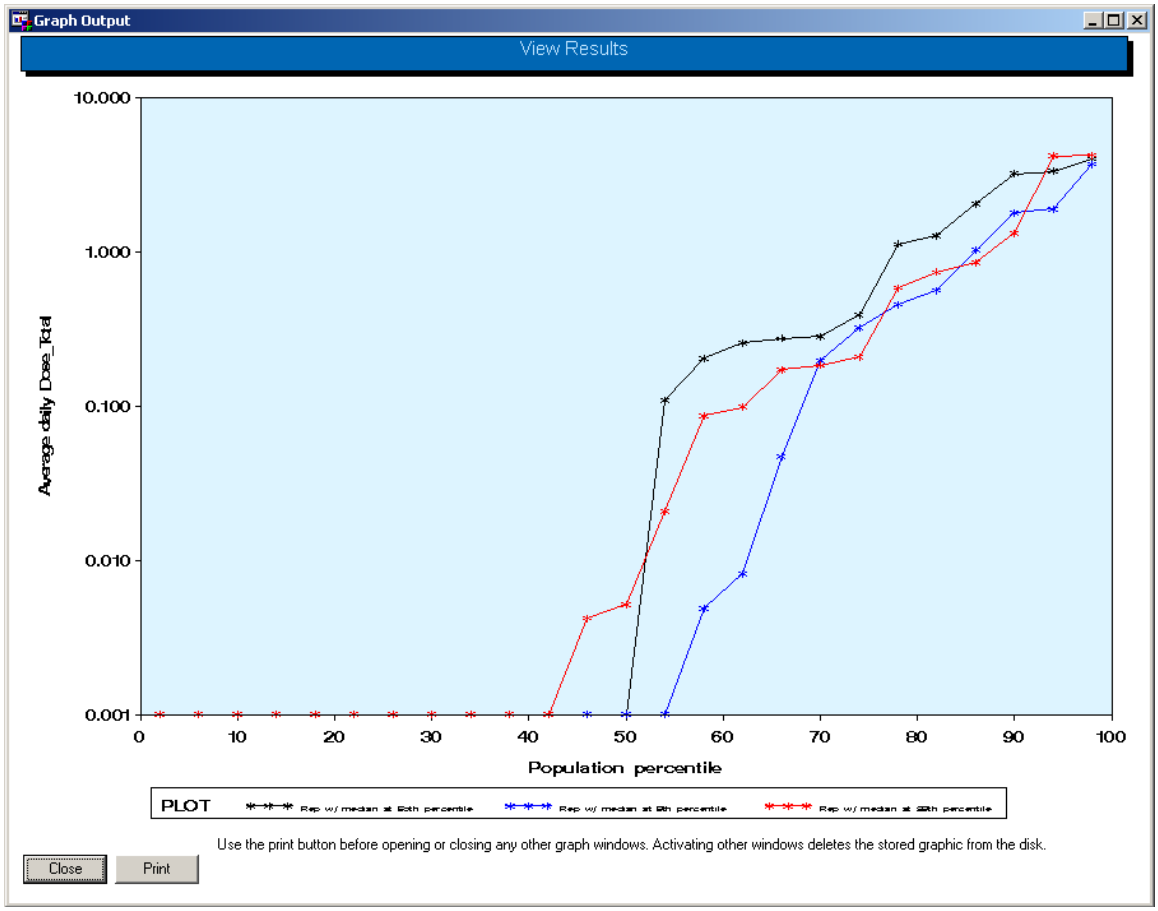


Figure 5.58. Plotting the CDFs from Uncertainty Repetitions whose Medians are at the 5th, 50th, and 95th Percentiles.

5.11.5 View Sensitivity Results

Selecting the View Sensitivity Results button from the View Results screen will open the window shown in Figure 5.59. This window allows the user to view a table of sensitivity results for the run. The format and contents of the table will vary based on the type of sensitivity run that was performed (Percentile Scaling, Sobol's Analysis, or Input-Output Correlation).

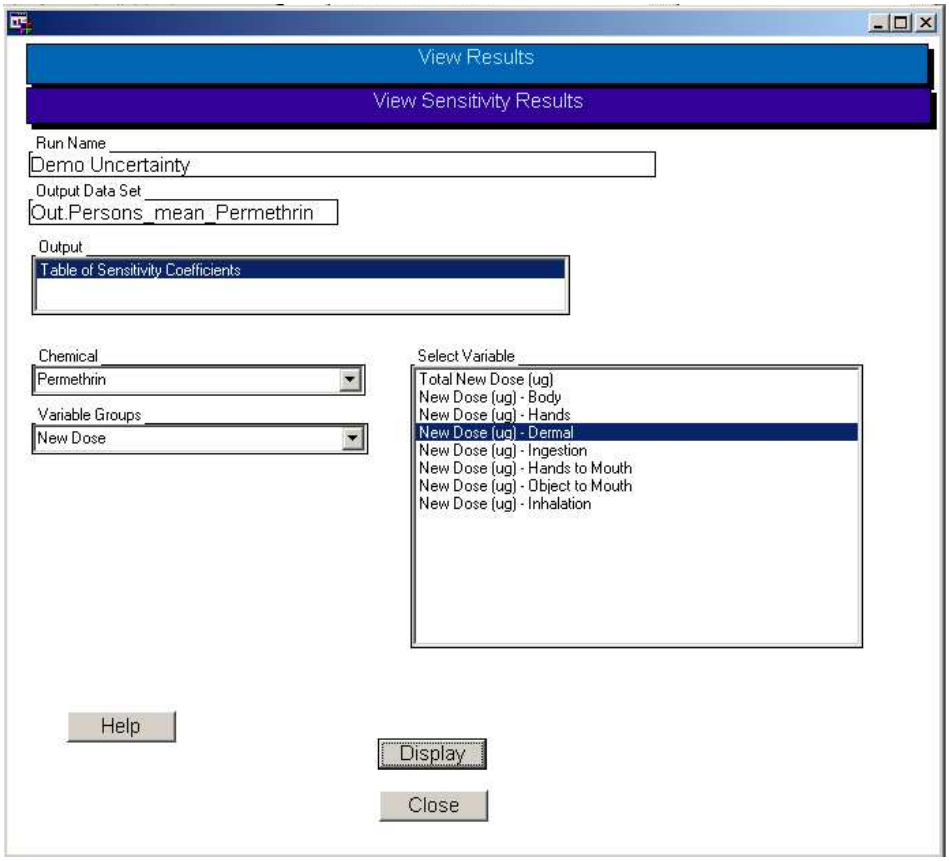


Figure 5.59. View Sensitivity Results Screen.

The user may select to view sensitivity results based on the population average of any model variable. The available variable groups are the same as described in Section 5.11.2 . The user specifies a variable group, a variable, and then clicks Display to view the sensitivity table.

5.11.5.1 Results for a Percentile Scaling Run

If a Percentile Scaling run was performed, the table of sensitivity results will resemble that shown in Figure 5.61. This table includes a list of all the model input variables in the run for which sensitivity was considered. (See Section 5.4.1 for information on how to specify a list of sensitivity inputs). Recall that a percentile scaling run performs a baseline (median) run with all the sensitivity inputs at their median values, and then repeats the run with each of the input values at a high and low percentile. (See the SHEDS Technical Manual for detailed information about the percentile scaling method.) The results of these runs are summarized in the table. The table contains the following information:

- **Variable.** The input variable name. For space reasons, the variables are listed by their short (code) names. See the SHEDS technical manual for a longer description of each variable.

- **Number of Persons.** The number of profiles in the run.

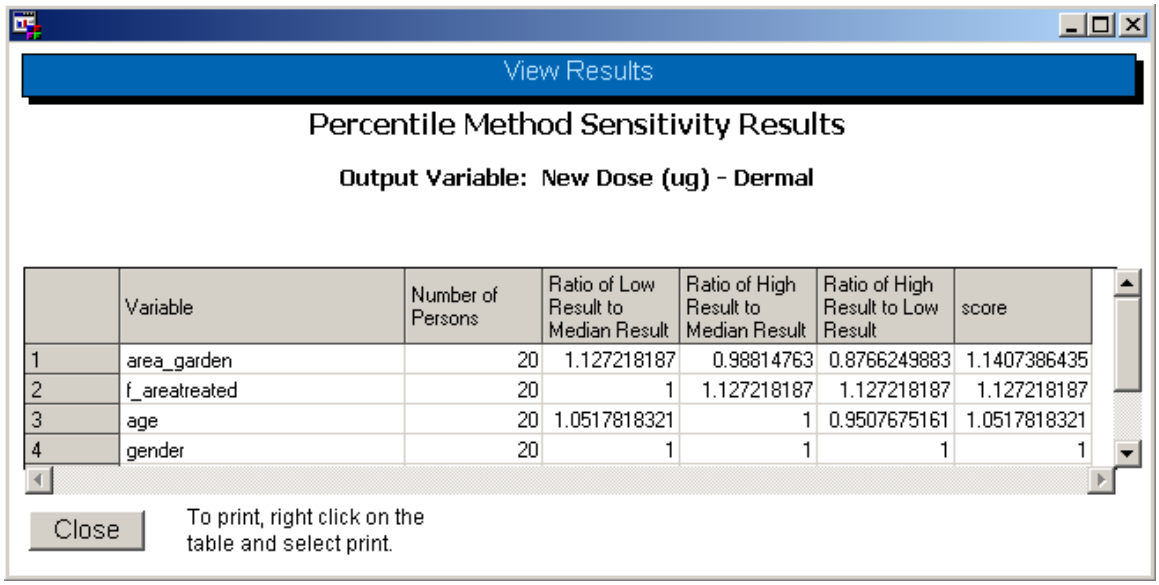
- **Ratio of Low Result to Median Result**. Ratio of the result for low-percentile run to that for the median run for the output variable selected.

- **Ratio of High Result to Median Result**. Ratio of the result for high-percentile run to that for the median run for the output variable selected.

- **Ratio of High Result to Low Result**. Ratio of the result for high-percentile run to that for low-percentile run.

- **Score.** A variable that indicates the relative difference between the high and low results for all input variables; it is equal to the Ratio of High Result to Low Result if this number is greater than 1, or its inverse if it is less than 1. It is used to rank the items in the table.

In the example shown in Figure 5.60, the sensitivity of the new dermal dose to four input variables was examined. Of the four variables being examined, the model was most sensitive to the area of the vegetable garden (area_garden). Note that this run is only for example purposes; many more profiles would be needed to develop real, useful sensitivity results.



	Variable	Number of Persons	Ratio of Low Result to Median Result	Ratio of High Result to Median Result	Ratio of High Result to Low Result	score
1	area_garden	20	1.127218187	0.98814763	0.8766249883	1.1407386435
2	f_areatreated	20	1	1.127218187	1.127218187	1.127218187
3	age	20	1.0517818321	1	0.9507675161	1.0517818321
4	gender	20	1	1	1	1

Figure 5.60. Sensitivity Results for a Percentile Scaling Run.

5.11.5.2 Results for a Sobol Sensitivity Run

An example of the sensitivity results for a Sobol run are shown in Figure 5.61. For this type of run, a number of output sensitivity variables are presented for each Sobol Group (see Section 5.4.1.2 for instructions on defining Sobol Groups). The output variables are as follows:

- **Main Effect.** The combined main effect of all the variables in the Sobol group.
- **Total Effect.** The combined total effect of all the variables in the Sobol group.
- **Percent of Total Variance.** The percent of the total variance in the output variable that is explained by variation in the variables in the Sobol group. This is calculated as the total effect of the group divided by sum of the total effect for all groups multiplied by 100.
- **Variables.** A list of the input variables in the Sobol group. For space reasons, the variables are listed by their short (code) names. See the SHEDS Technical Manual for a longer description of each variable.

Note that it may require large numbers of profiles to be run to capture adequately the sensitivity of the model to the Sobol groups. In this example, the fact that a total effect of greater than 1 was found indicates that there is considerable uncertainty in these estimates. See the SHEDS Technical Manual for details on performing Sobol runs.

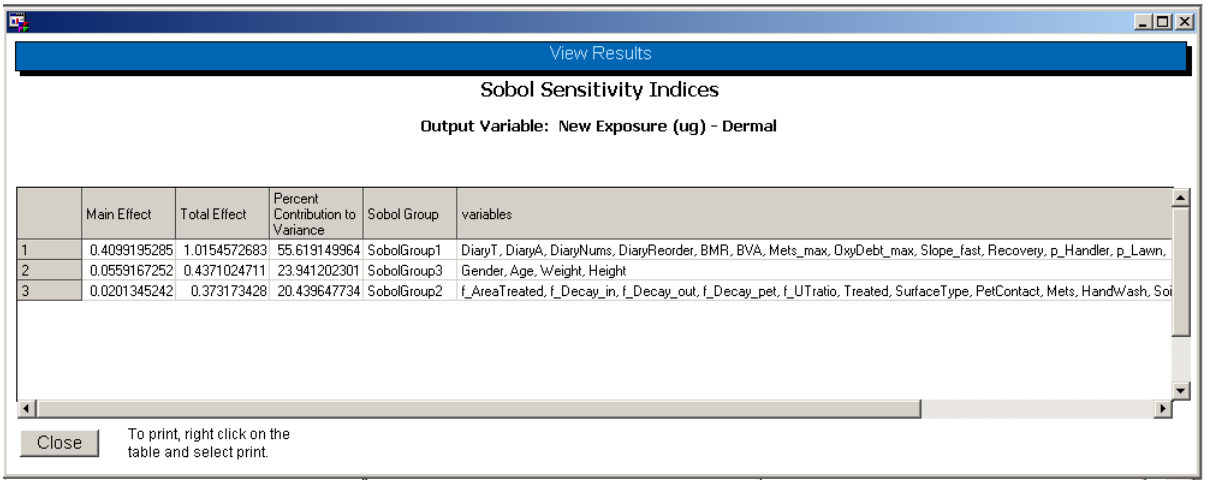
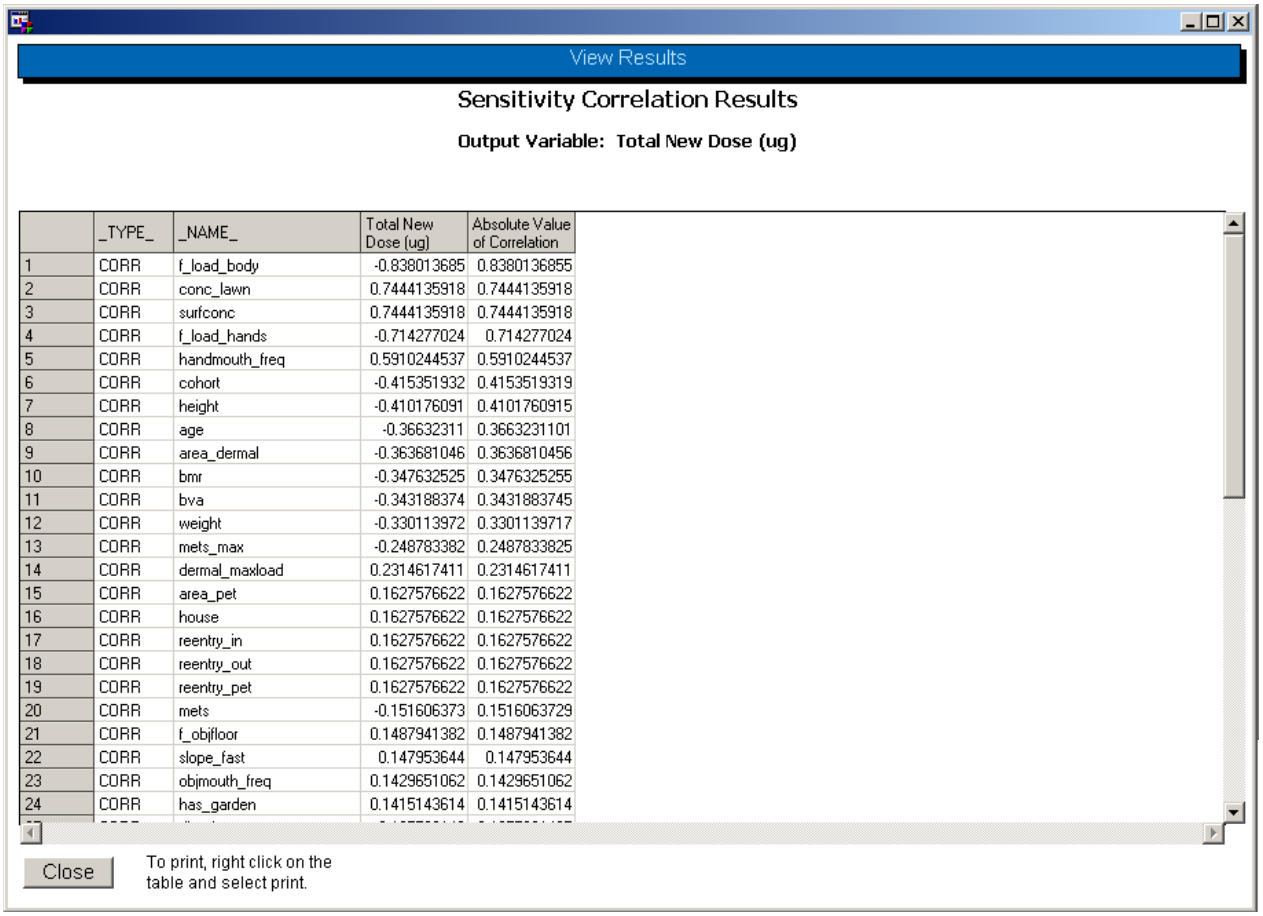


Figure 5.61. Sensitivity Results for a Sobol Analysis Run.

5.11.5.3 *Results for a Input-Output Correlation Sensitivity Run*

If the type of sensitivity analysis being performed is an input-output correlation run, the table of sensitivity results will be similar to that shown in Figure 5.62. This table contains a list of all the input variables in the run, and their correlation with the selected variable (Total New Dose in the example in Figure 5.62). The absolute value of this correlation is also given. It is used to determine the order of the variables in the table; variables with the highest correlations with the output variable will be at the top of the table. For space reasons, the variables are listed by their short (code) names. See the SHEDS Technical Manual for a longer description of each variable and for more information about calculating input-output correlations.

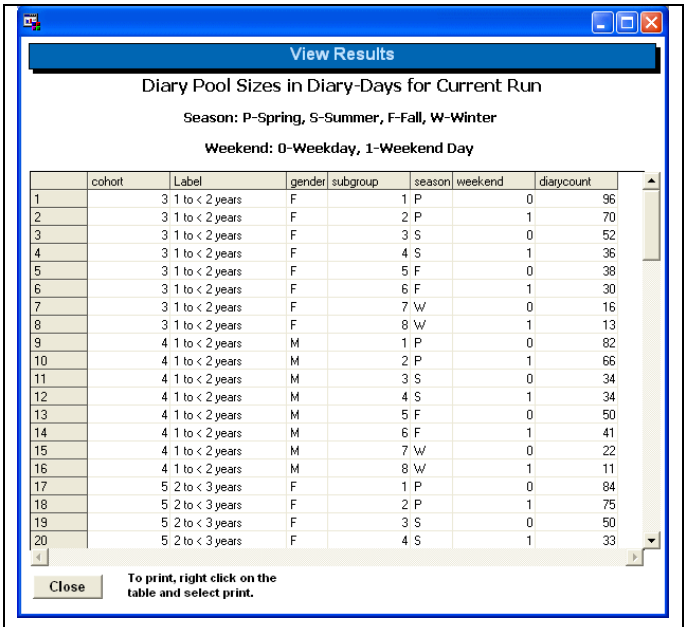


	TYPE	_NAME_	Total New Dose (ug)	Absolute Value of Correlation
1	CORR	f_load_body	-0.838013685	0.8380136855
2	CORR	conc_lawn	0.7444135918	0.7444135918
3	CORR	surfconc	0.7444135918	0.7444135918
4	CORR	f_load_hands	-0.714277024	0.714277024
5	CORR	handmouth_freq	0.5910244537	0.5910244537
6	CORR	cohort	-0.415351932	0.4153519319
7	CORR	height	-0.410176091	0.4101760915
8	CORR	age	-0.36632311	0.3663231101
9	CORR	area_dermal	-0.363681046	0.3636810456
10	CORR	bmr	-0.347632525	0.3476325255
11	CORR	bva	-0.343188374	0.3431883745
12	CORR	weight	-0.330113972	0.3301139717
13	CORR	mets_max	-0.248783382	0.2487833825
14	CORR	dermal_maxload	0.2314617411	0.2314617411
15	CORR	area_pet	0.1627576622	0.1627576622
16	CORR	house	0.1627576622	0.1627576622
17	CORR	reentry_in	0.1627576622	0.1627576622
18	CORR	reentry_out	0.1627576622	0.1627576622
19	CORR	reentry_pet	0.1627576622	0.1627576622
20	CORR	mets	-0.151606373	0.1516063729
21	CORR	f_objfloor	0.1487941382	0.1487941382
22	CORR	slope_fast	0.147953644	0.147953644
23	CORR	objmouth_freq	0.1429651062	0.1429651062
24	CORR	has_garden	0.1415143614	0.1415143614

Figure 5.62. Sensitivity Results for an Input-Output Correlation Run.

5.11.6 View Diary Pool Sizes

Activity diaries are selected at random from pools that are characterized by different personal and temporal characteristics. Figure 5-39 provides an example of counts of diaries available for each diary pool as determined by the user's inputs for the simulations. The user is reminded that larger diary pools better represent the population.



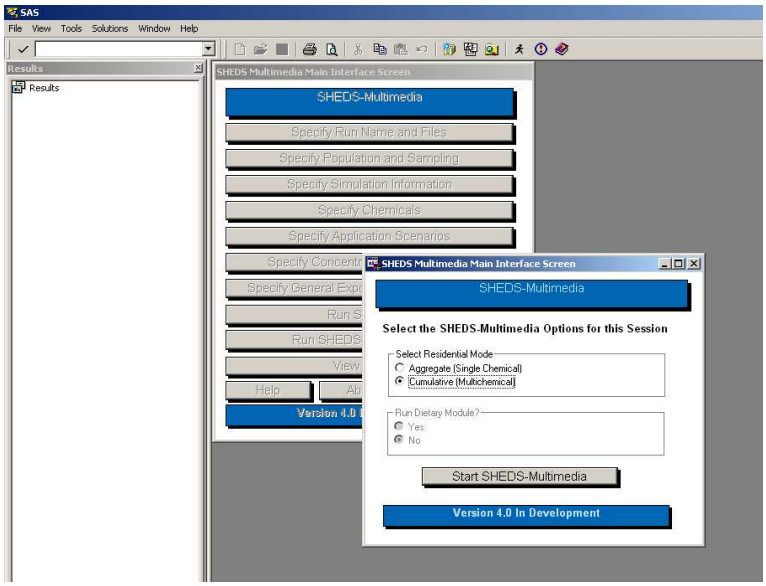
	cohort	Label	gender	subgroup	season	weekend	diarycount
1	3	1 to < 2 years	F	1	P	0	96
2	3	1 to < 2 years	F	2	P	1	70
3	3	1 to < 2 years	F	3	S	0	52
4	3	1 to < 2 years	F	4	S	1	36
5	3	1 to < 2 years	F	5	F	0	38
6	3	1 to < 2 years	F	6	F	1	30
7	3	1 to < 2 years	F	7	W	0	16
8	3	1 to < 2 years	F	8	W	1	13
9	4	1 to < 2 years	M	1	P	0	82
10	4	1 to < 2 years	M	2	P	1	66
11	4	1 to < 2 years	M	3	S	0	34
12	4	1 to < 2 years	M	4	S	1	34
13	4	1 to < 2 years	M	5	F	0	50
14	4	1 to < 2 years	M	6	F	1	41
15	4	1 to < 2 years	M	7	W	0	22
16	4	1 to < 2 years	M	8	W	1	11
17	5	2 to < 3 years	F	1	P	0	84
18	5	2 to < 3 years	F	2	P	1	75
19	5	2 to < 3 years	F	3	S	0	50
20	5	2 to < 3 years	F	4	S	1	33

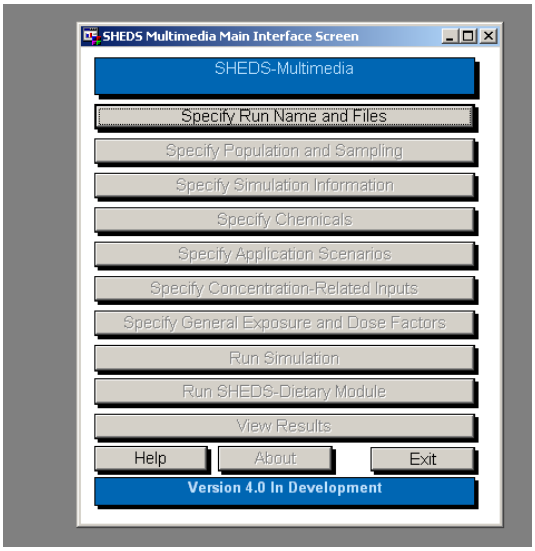
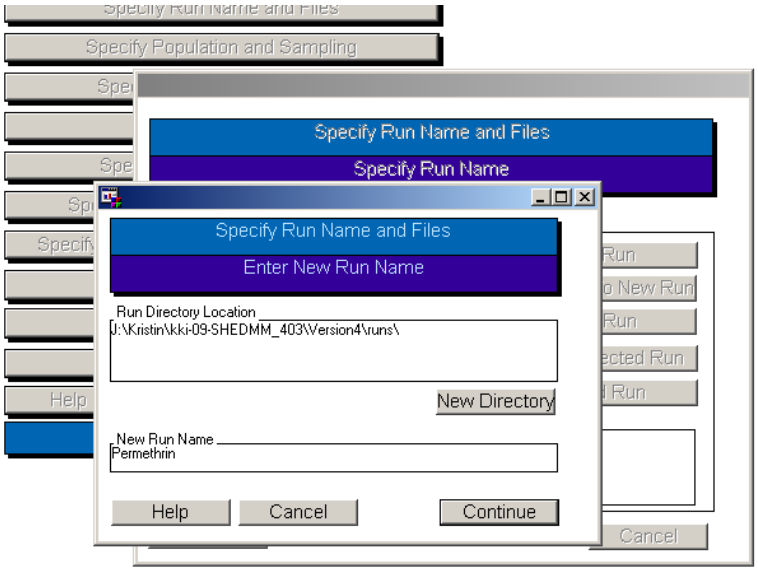
Figure 5.63. Example Diary Pool Size Table.

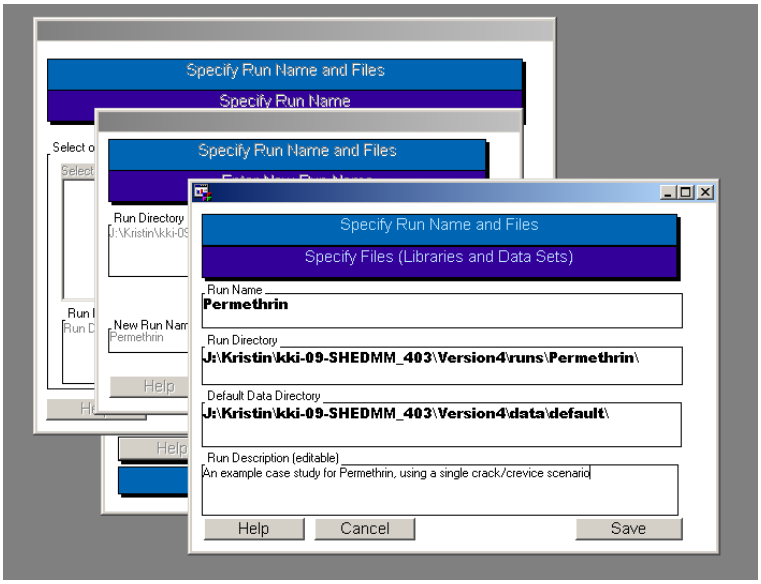
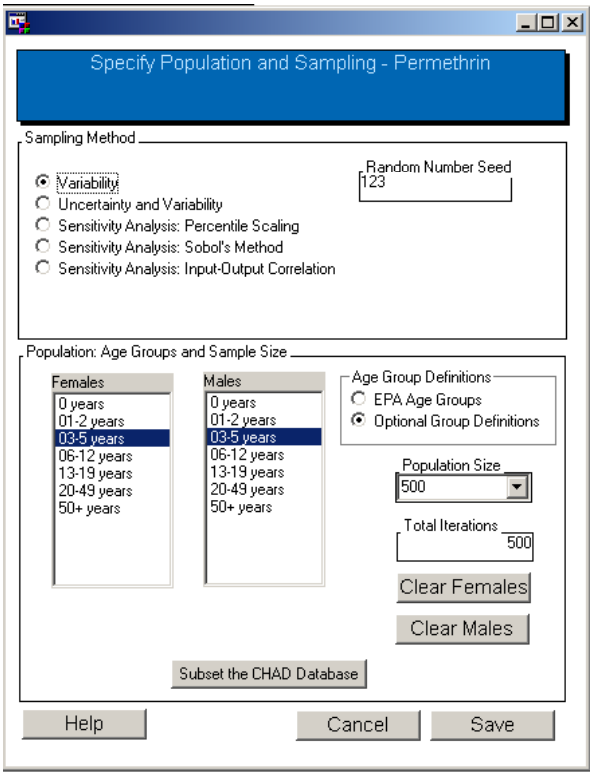
6 Case Study: Permethrin

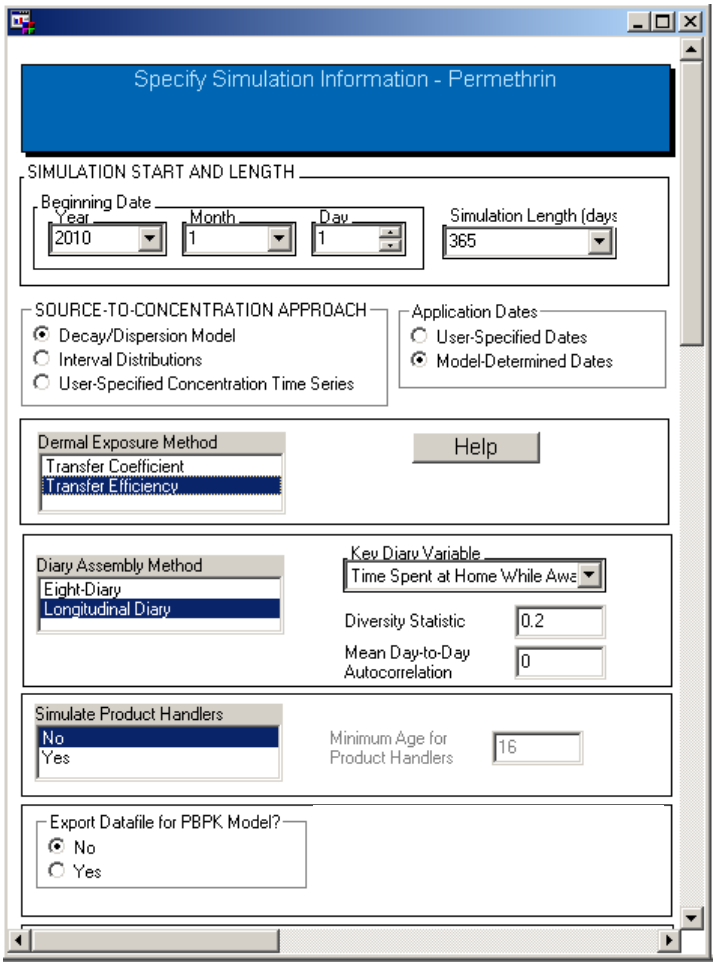
This chapter provides an example of creating a SHEDS-Residential run from start to finish. The run presented herein is a single-chemical variability run for Permethrin. The run considers a single application scenario (an indoor crack-crevice aerosol); the application dates are model-determined. This example run is included in the SHEDS-Residential installation; it will be available for selection when Edit an Existing Run is selected under the name Permethrin Case Study. However, the steps presented here show the user how to create the run from scratch. Each step in creating the run will be illustrated with an accompanying screenshot.

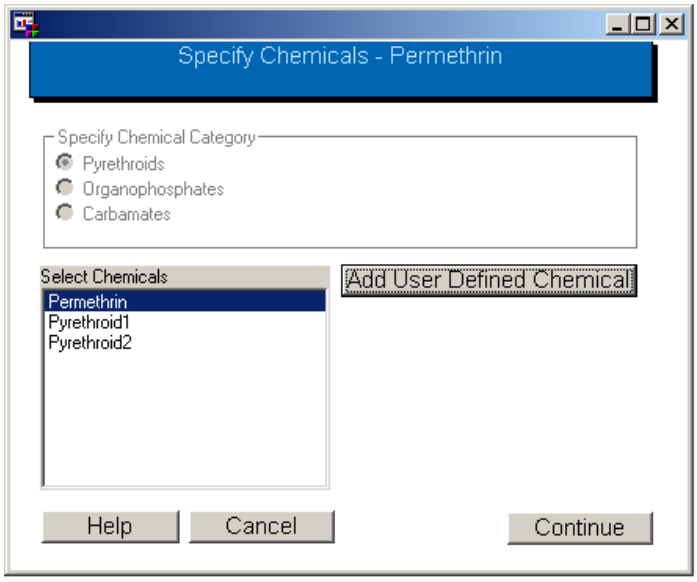
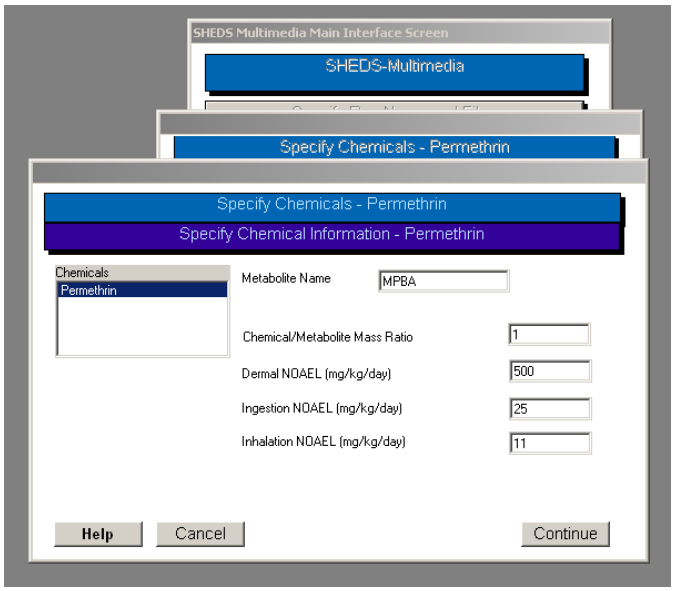
Note: Since SHEDS is in development, the results seen here may differ from that seen by the user.

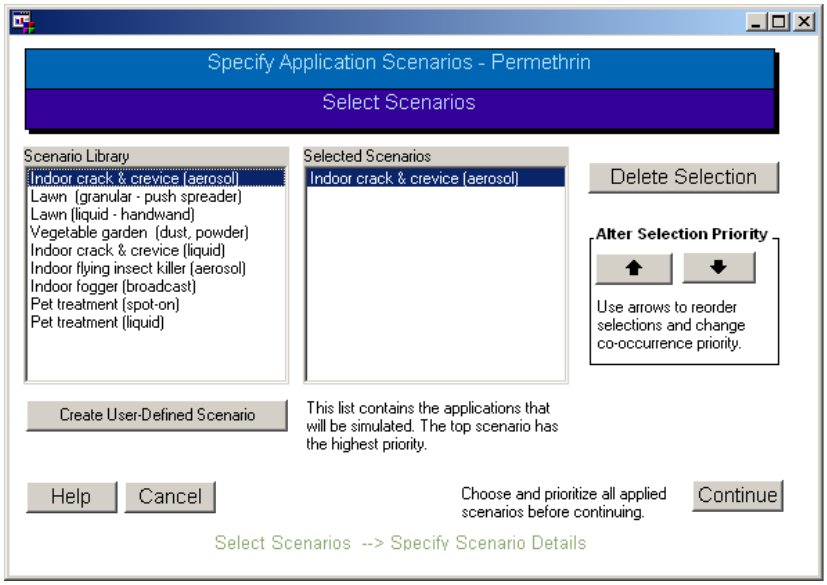
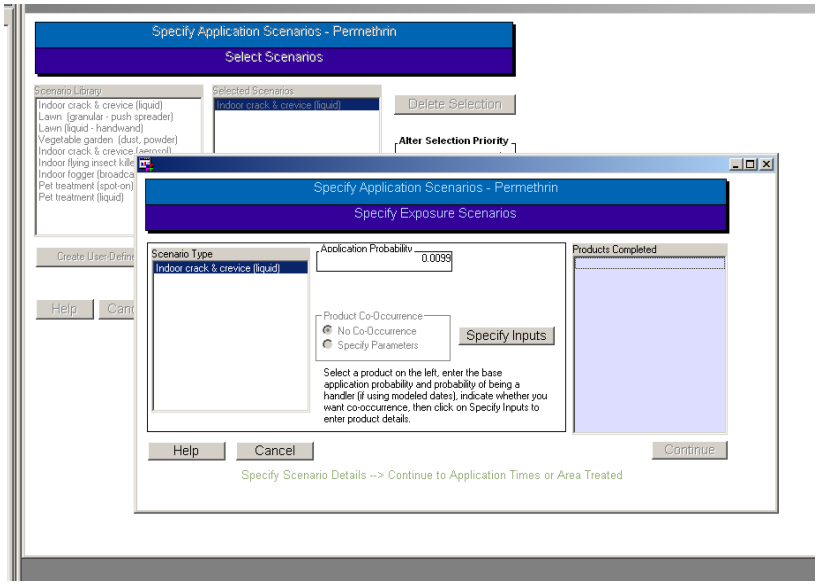
Start the SHEDS-Residential interface. Select Cumulative Mode. Although this is a single-chemical run, this example will step through the Cumulative Model screens so the user can see the steps they would need to complete for a multichemical run. Click <Start \SHEDS-Residential>.	

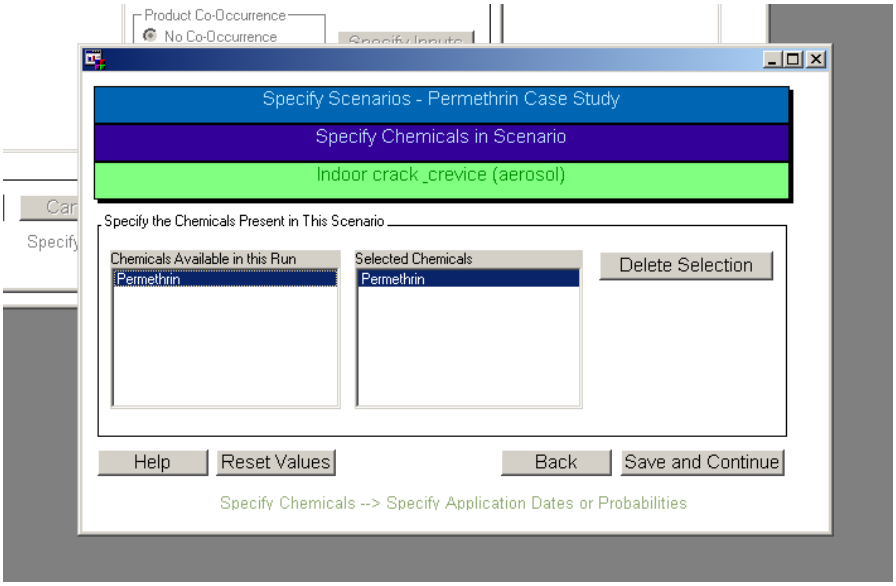
Click <Specify Run Name and Files>.	
Click <Create a New Run >. Enter a name for the run, in this case, “Permethrin.” Click <Continue>. The location of the information for the run (input and output) can be changed on this screen, if desired.	

Enter a description for the run, if desired (this is optional). Click <Save>.	
Click <Specify Population and Sampling>. The run type "Variability" will be selected by default. Select "Optional Group Definitions," and choose to run males and females 3-5 years of age by highlighting the age groups. Enter a population size of 500 profiles (this can be directly typed in, or the arrows can be used to select common population sizes). (The number of total iterations is automatically updated). Click <Save>.	

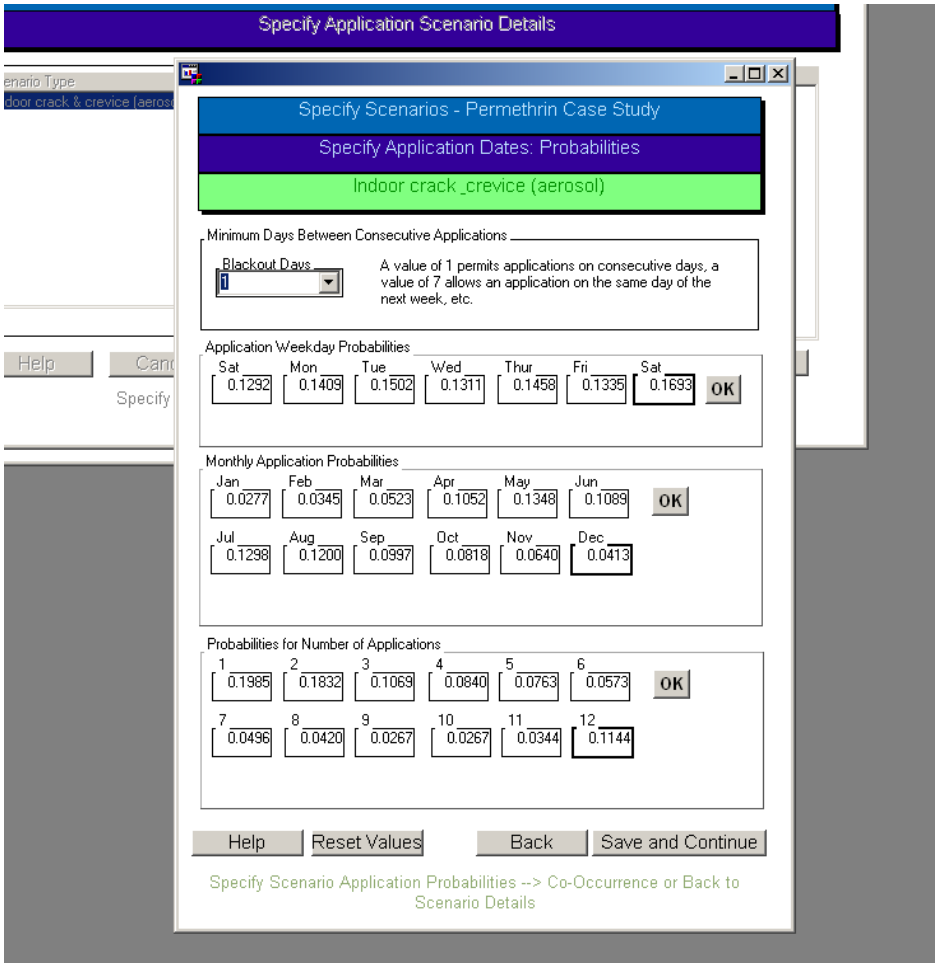
Click on <Specify Simulation Information> on the Main screen. Select January, 1, 2010 as the start date and enter 365 as the number of days in the year. Select "Model-Determined Dates" as the Application Dates method. Select "Transfer Efficiency" as the dermal exposure method. For the Diary Assembly method, highlight "Longitudinal Diary." This will enable the key variable, diversity, and autocorrelation widgets. Select "Time Spent at Home While Awake" as the key variable, 0.2 as the diversity statistic, and 0 for mean day-to-day autocorrelation. Leave other variables at defaults, and Click <Save>.	

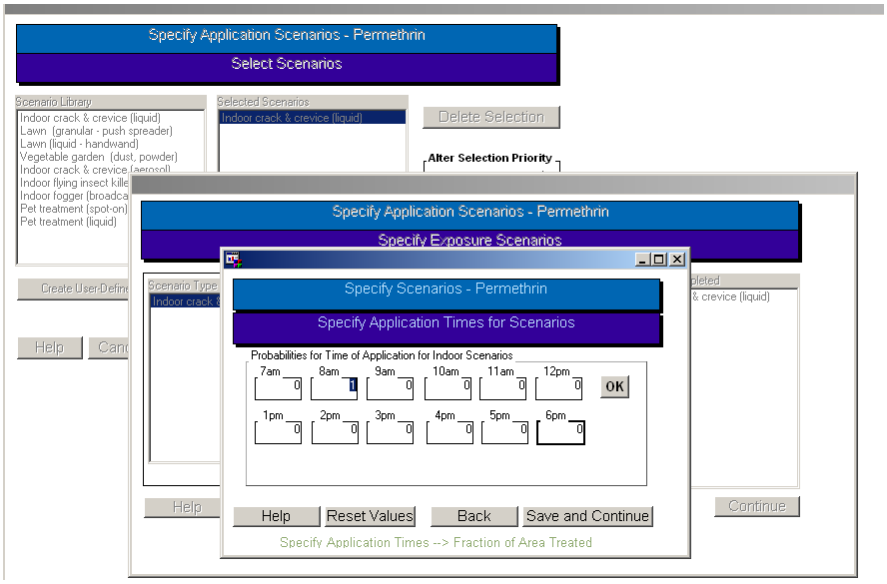
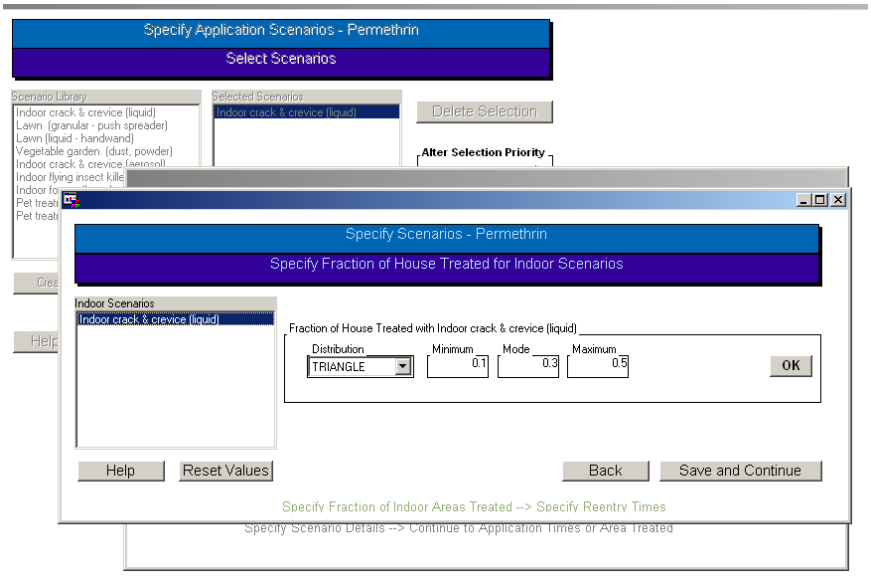
Click <Specify Chemicals> on the main screen. Choose to model Permethrin by highlighting it (and only it) in the Select Chemicals list box. Chemicals can be toggled between selected/unselected by clicking on them in the list box. Click <Continue>.	
Accept the default values for Permethrin on the Specify Chemical Information screen by clicking <Continue>. This will return the user to the main screen.	

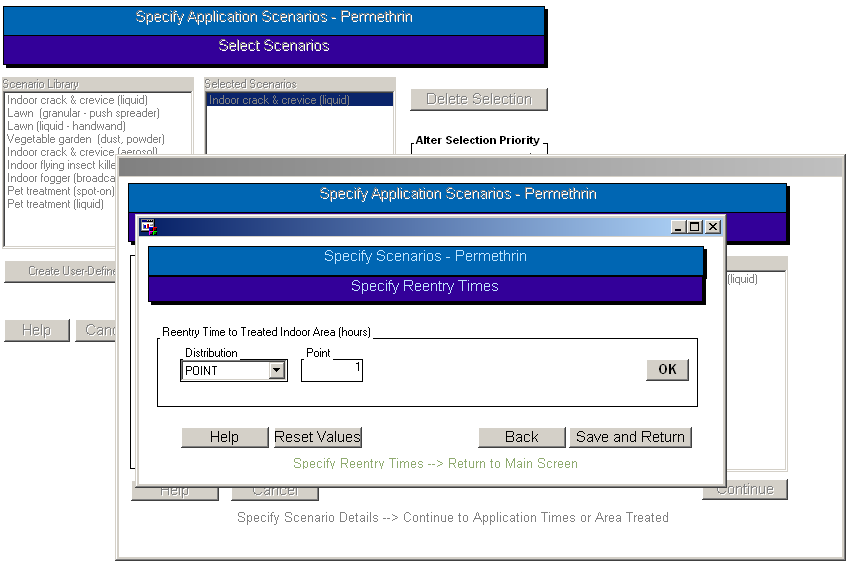
Click <Specify Application Scenarios> on the Main Screen. This will open the Select Scenarios screen. Select "Indoor Crack and Crevice (aerosol)" from the Scenario Library. When the scenario appears in the Selected Scenarios box, click <Continue> to move to the Specify Scenario Details screen.	
Click <Specify Inputs> to enter information for the crack/crevice scenario.	

The first scenario screen is the Specify Chemicals in Scenario screen. Click on Permethrin to add the chemical to the scenario. In Aggregate mode, this screen is skipped because the model assumes the single chemical will be present in the scenario. If more than one chemical were available, the user could assign a subset of the chemicals to each scenario. Click <Save and Continue> to proceed.	

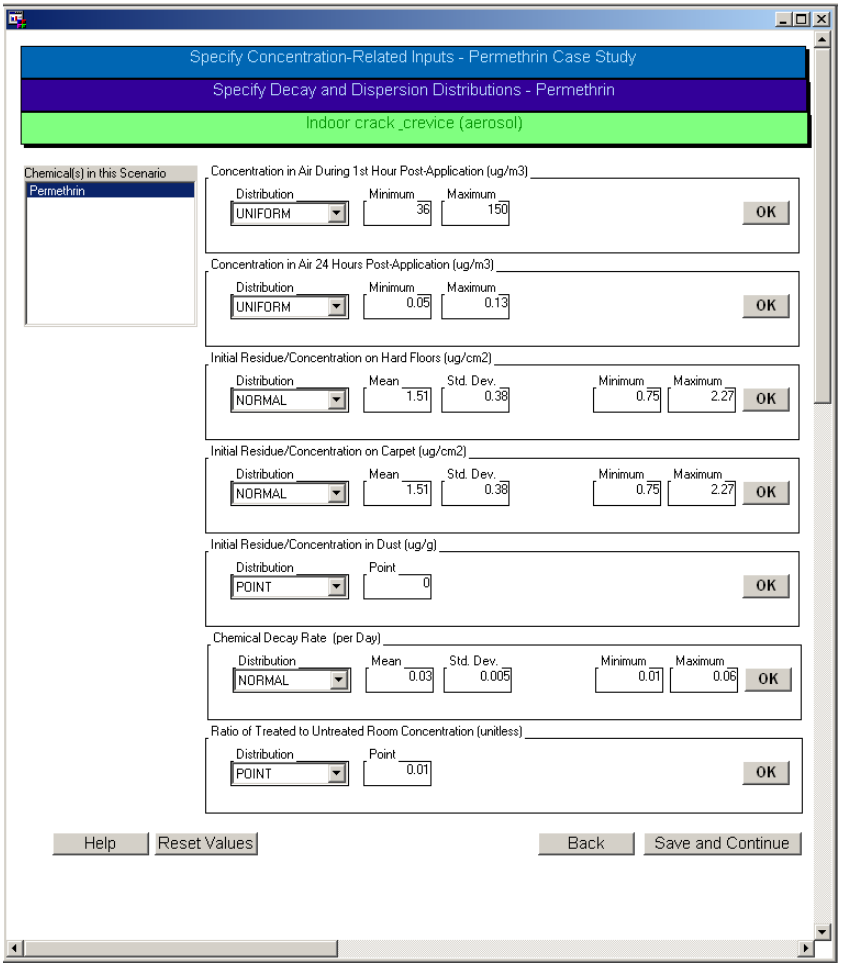
The next screen in the scenario cascade is the Application Probabilities screen. Accept the defaults by clicking <Save and Continue>. This returns the user to the Specify Scenarios Screen. Click <Continue> again to proceed.

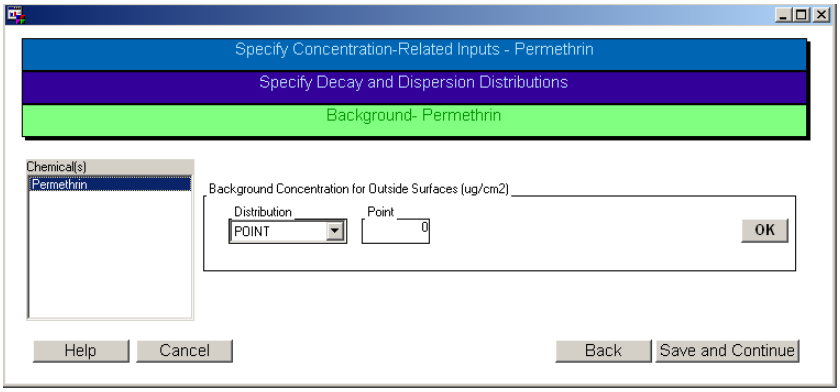
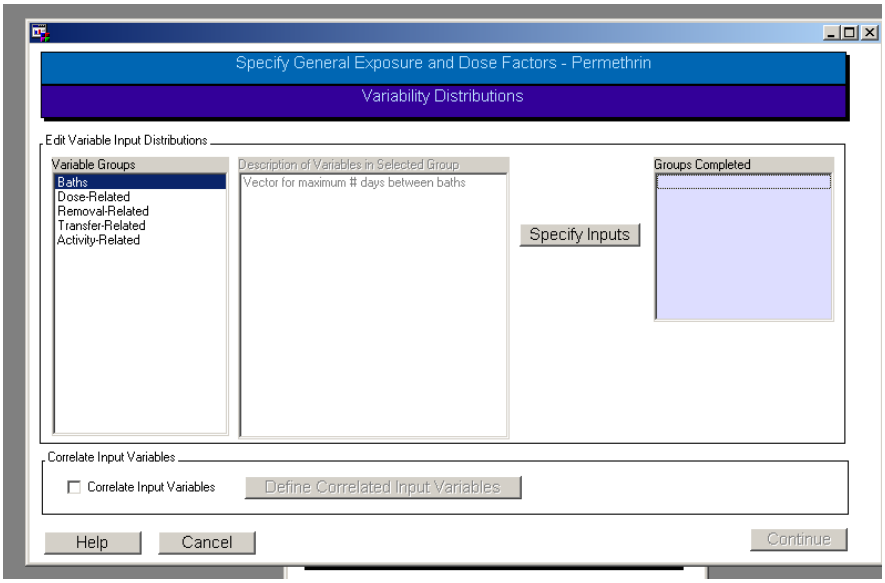


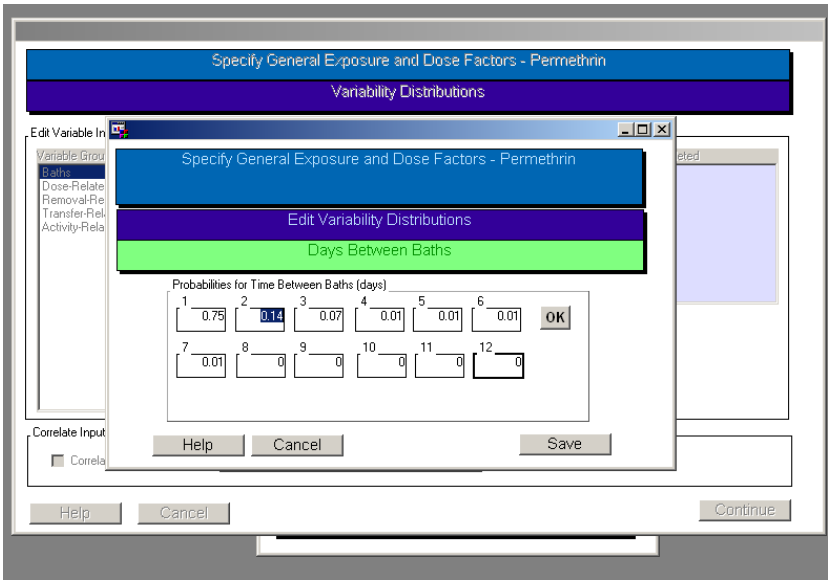
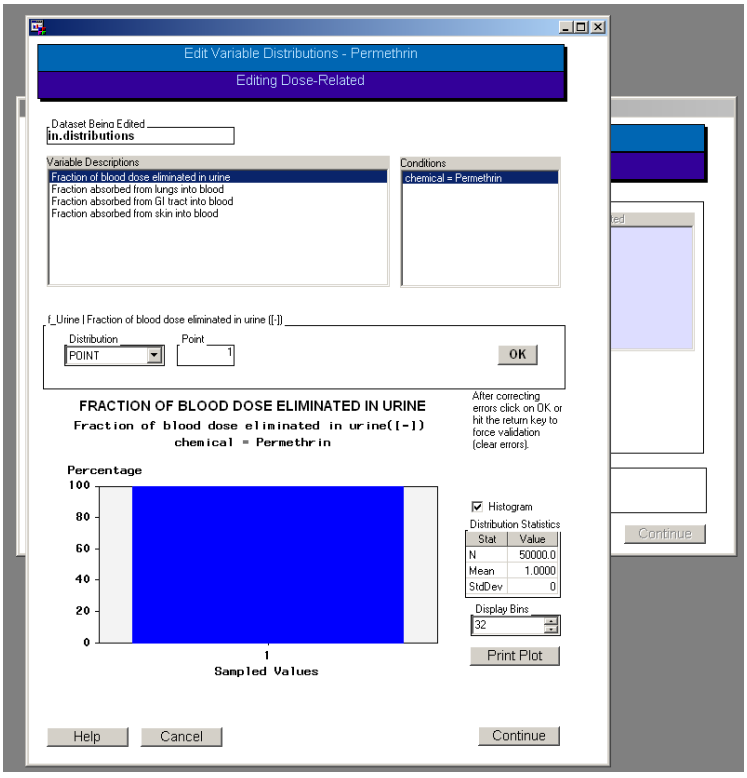
The next screen is the Application Times screen, where the user specifies a probability vector for the time of application of the chemical for any indoor scenarios. Accept the defaults by clicking <Save and Continue>.	
The next screen appears only when an indoor scenario is included in the run. Accept the default fraction of the house treated with the crack/crevice aerosol by clicking <Save and Continue>. This proceeds to the Re-entry screen.	

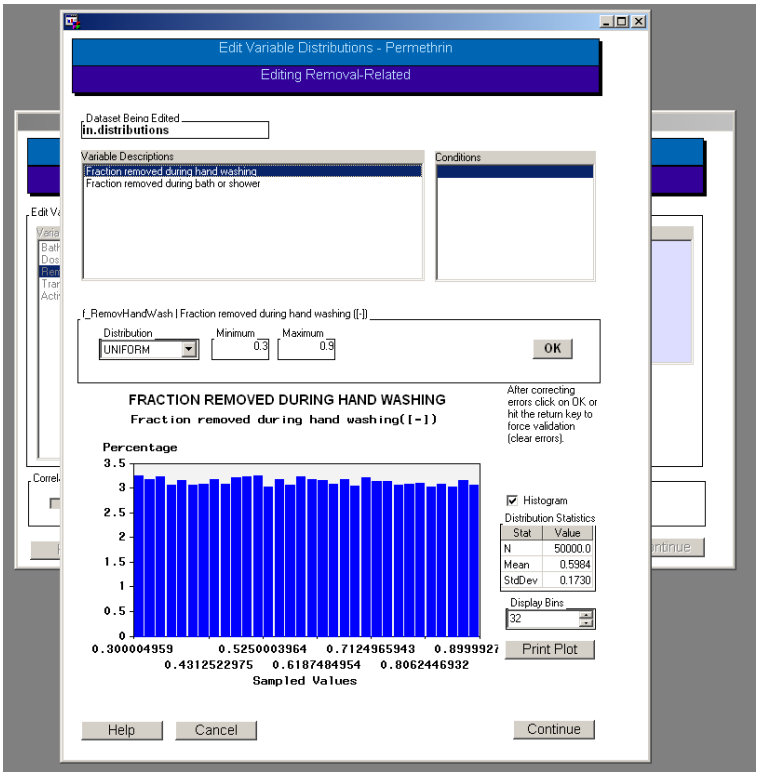
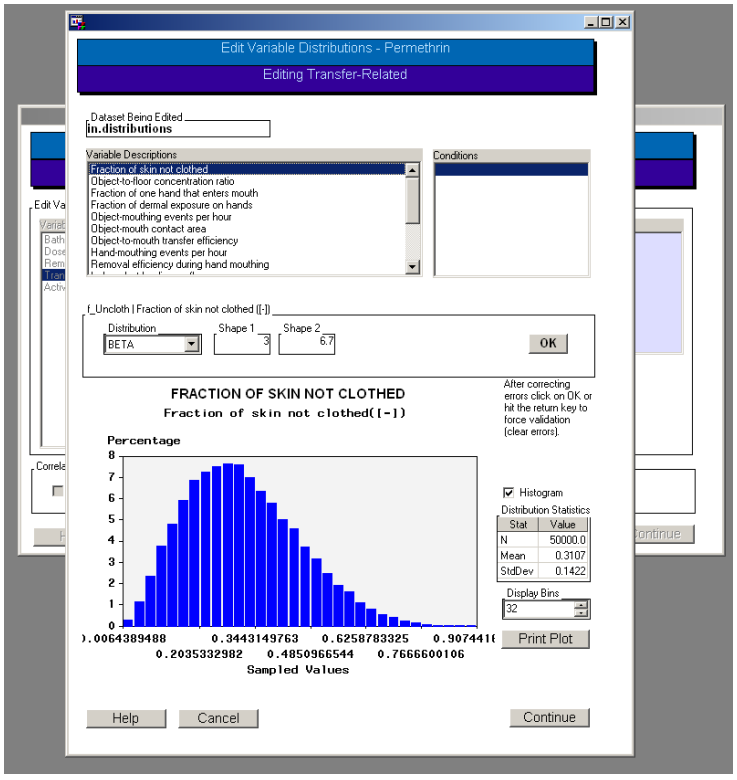
Only a re-entry time for indoor areas is available because this run only includes a single indoor scenario. If outdoor or pet scenarios were included in the run, this screen would contain more distributions to specify. Click <Save and Return> to accept the default re-entry time and return to the Main screen.	

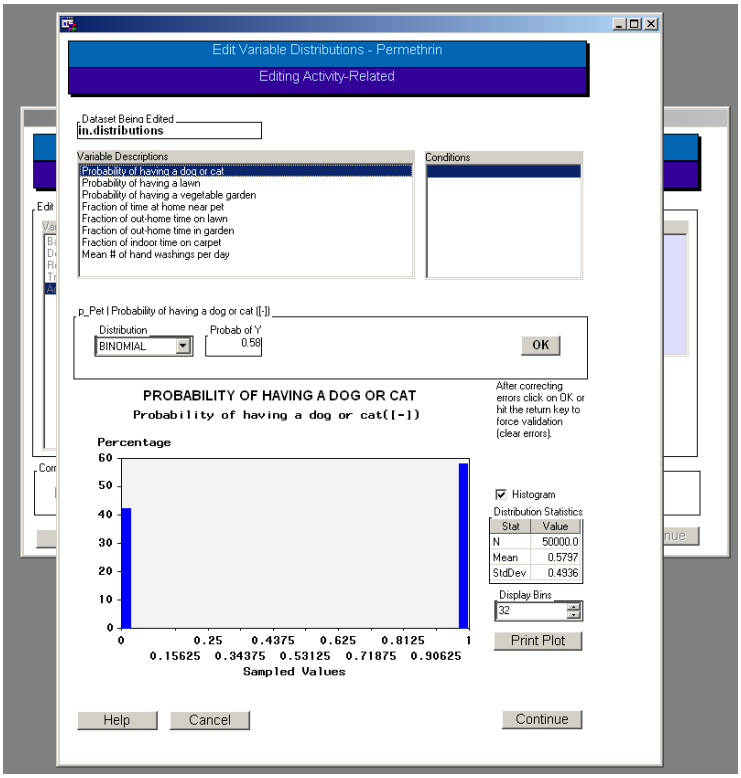
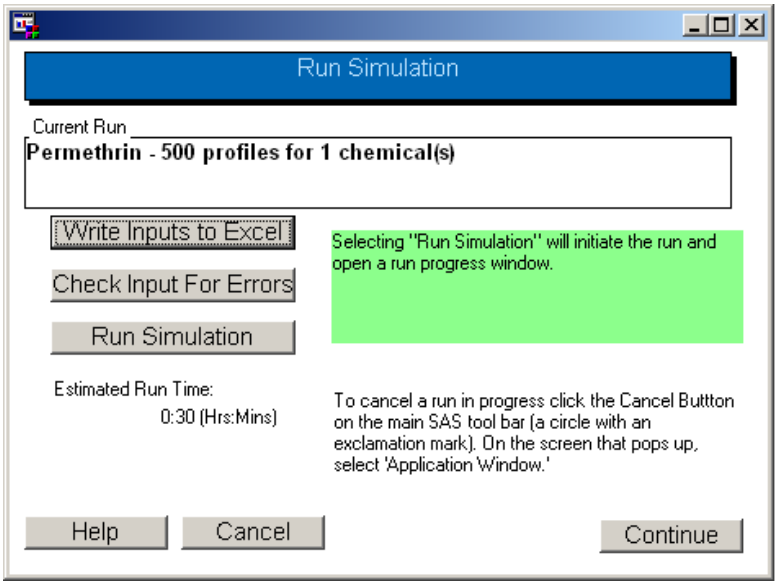
Click on <Concentration Related Inputs> on the main screen. This initiates the Concentration screen cascade. After a warning related to chemical transfer, the first screen is the Decay and Dispersion Distributions. This screen is present because Decay and Dispersion was selected as the Source-to-Concentration Approach earlier in the run. Note that these variables are chemical-dependent; if there were more than one chemical present in the run, they would be included in the list box on the left side of the screen. Click <Save and Continue> to accept the defaults for Permethrin.

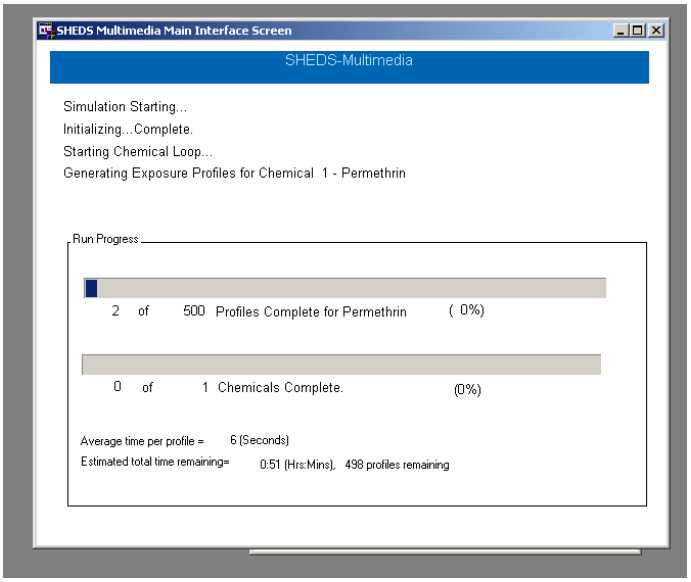
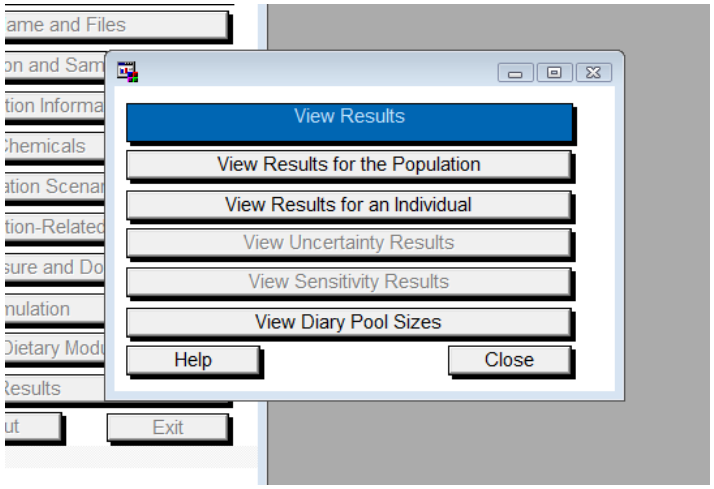


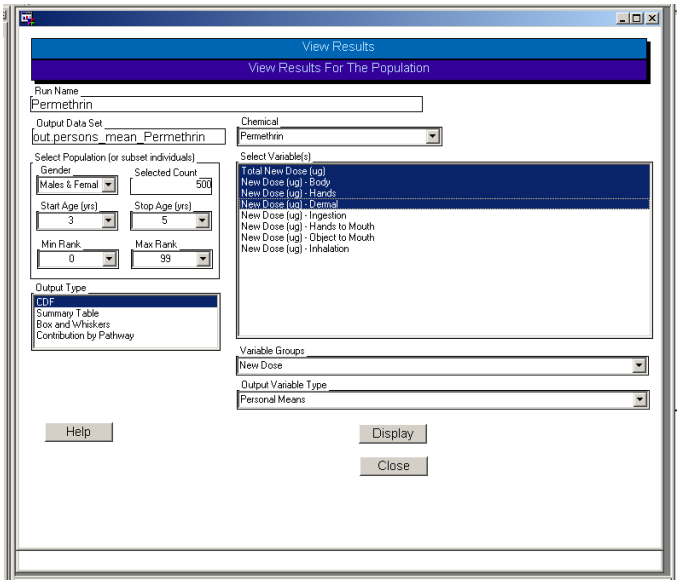
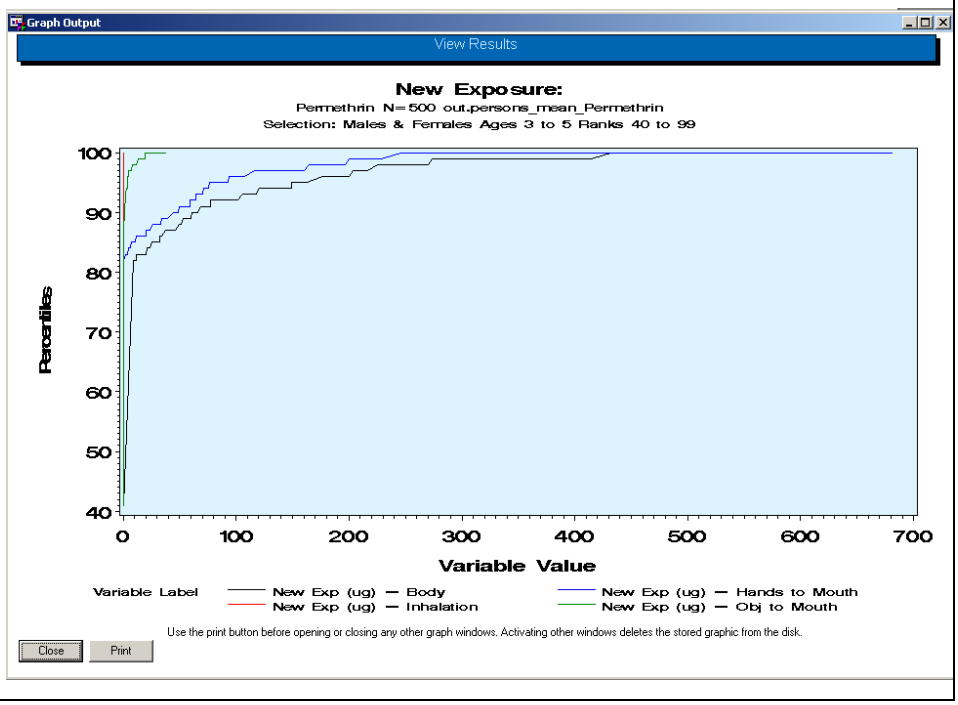
Click <Save and Continue> to accept the default value of 0 for permethrin background concentration. This returns the user to the Main screen.	
Click <Specify General Exposure and Dose Variables> on the Main screen. This opens the Variability Distributions screen. The user will need to visit each of the variable groups before being allowed to continue. Click <Specify Inputs> to view/edit the Baths variable group.	

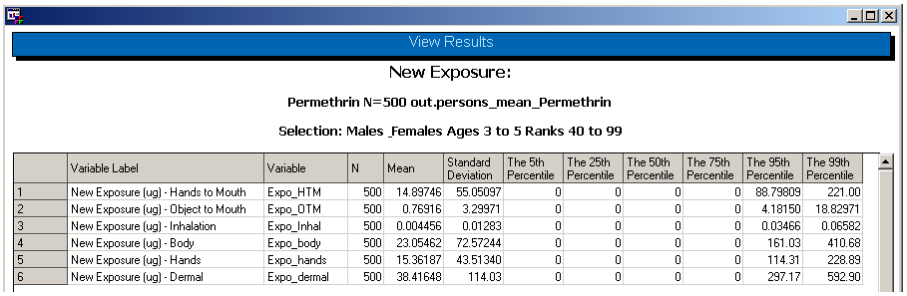
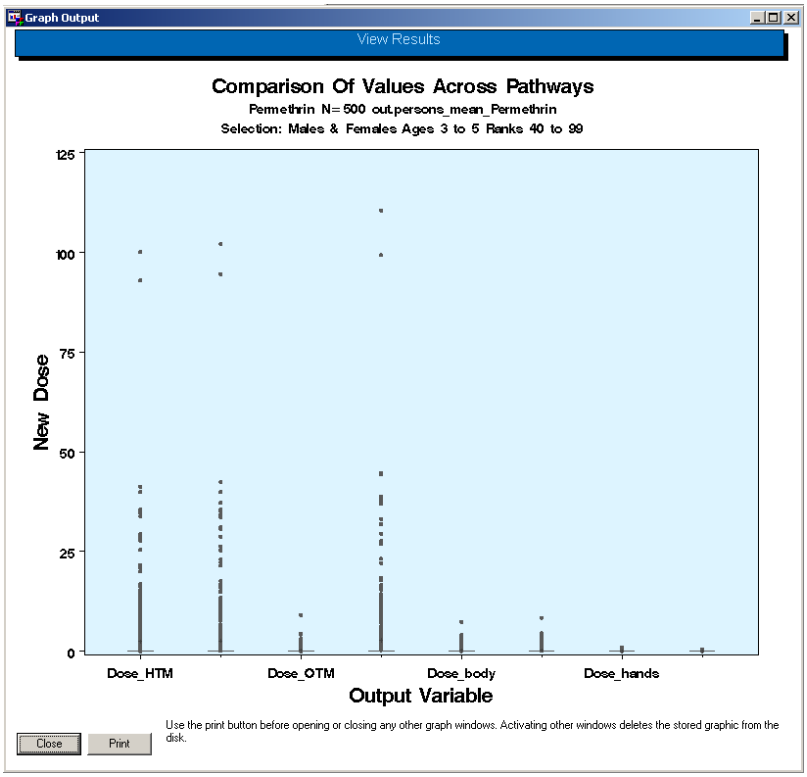
The Baths group is a special case: it consists of a single probability vector for days between baths. Accept the defaults by clicking <Save>.	
When the user is returned to the prior screen, the next Variable group, “Dose-Related,” should be highlighted. Click <Specify Inputs> again to edit this group. This opens the Edit Variable Distributions window, which allows the user to view or edit any of the distributions in the group, for any available conditions. Click <Continue> to accept the defaults for permethrin and return to the prior screen.	

Click <Specify Inputs> to edit variables in the "Removal-Related" group. Click <Continue> to accept the defaults and return to the prior screen.	
Click <Specify Inputs> to edit variables in the "Transfer-Related" group. Click <Continue> to accept the defaults and return to the prior screen.	

Click <Specify Inputs> to edit variables in the "Activity-Related" group. Click <Continue> to accept the defaults and return to the prior screen. Then click <Continue> once more to return to the Main screen.	
Click <Run Simulation> on the Main screen. This brings up the Run Simulation Screen. The screen should indicate that 500 profiles will be run for one chemical. Click <Run Simulation> to initiate the simulation.	

This opens the SHEDS-Residential Run Progress screen. This gives the user an idea how long the simulation will take to complete. This run should take between 20 minutes and an hour depending on the age/configuration of the user's computer. When the run is complete, this window will close automatically and return to the Run screen. Click <Continue> to return to the Main screen.	
Select <View Results> from the Main screen. Then click <View Results for the Population>.	

Select “New Dose” as the variable group, then Select “Total New Dose”, and the New Dose variables for “Hands”, “Body”, and “Dermal” from the available variables. Click <Display> to view the default output type, CDF.	
This draws a plot with CDFs for the 4 variables that were selected. Click <Close> to return to View Results for the Population.	

Select “Summary Table” as the output type. Select “New Exposure” as the variable group, highlight all the available variables, and click <Display>. This creates the table. Click<Close> to return to the previous screen.	
Select “Box and Whiskers” as the output type. Select “New Dose Normalized to Body Mass” as the variable group, highlight all the available variables, and click <Display>. This creates the box plot. Click<Close> to return to the previous screen.	

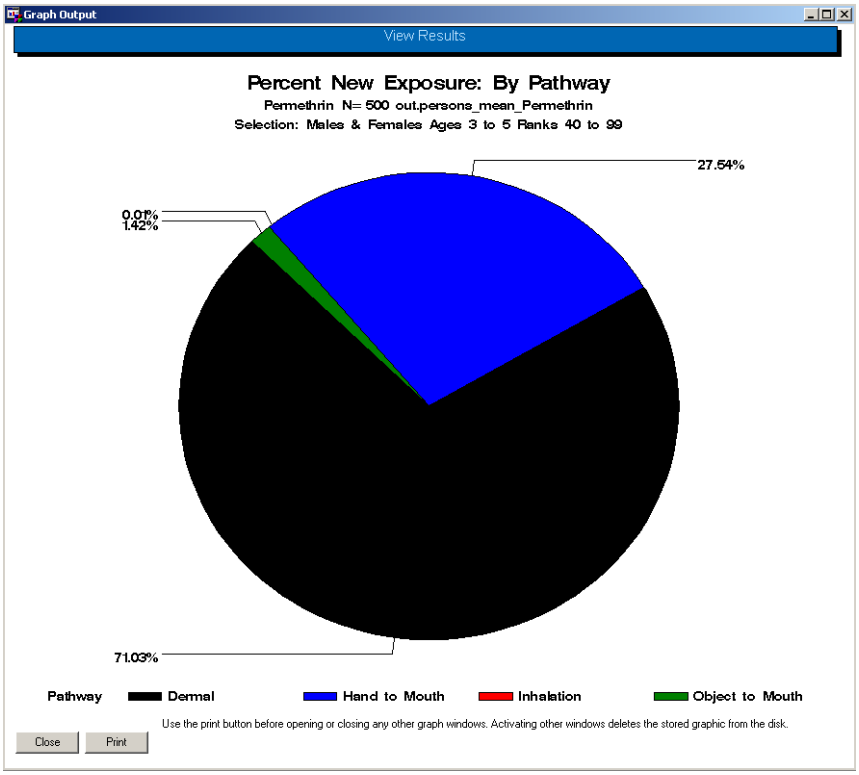
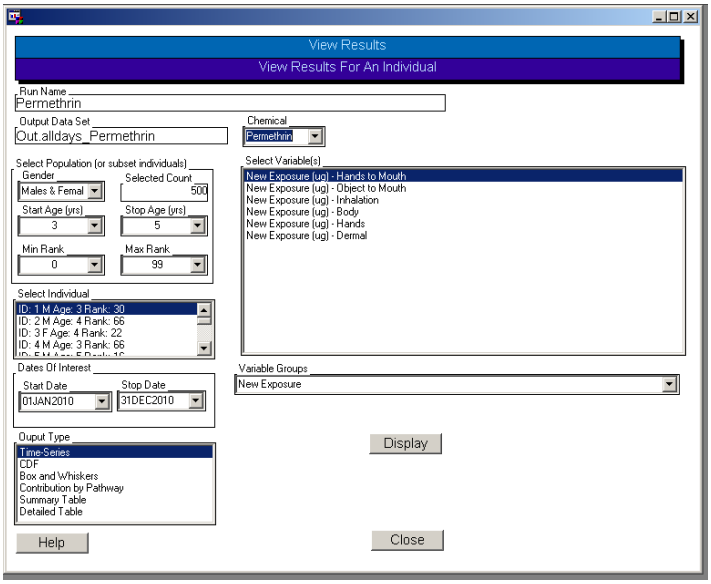
View Results

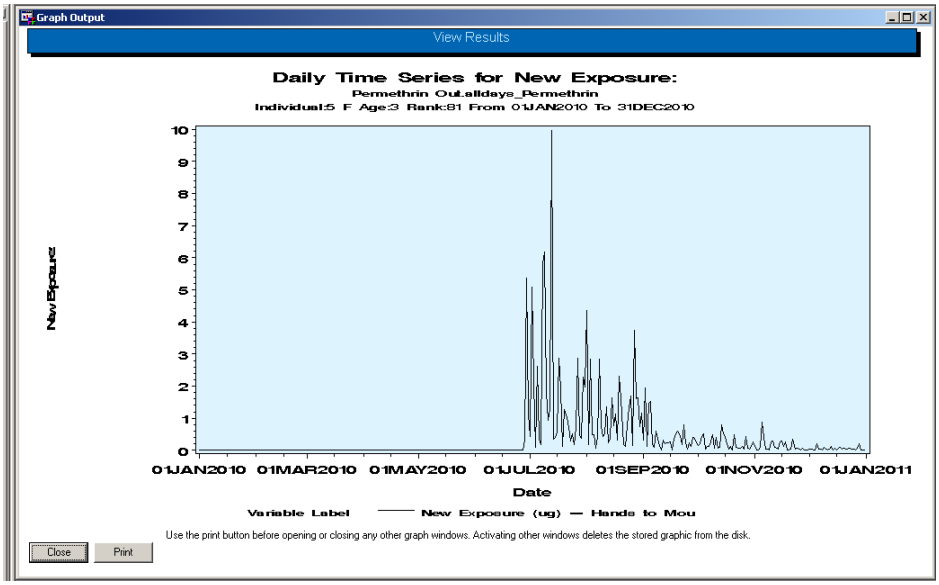
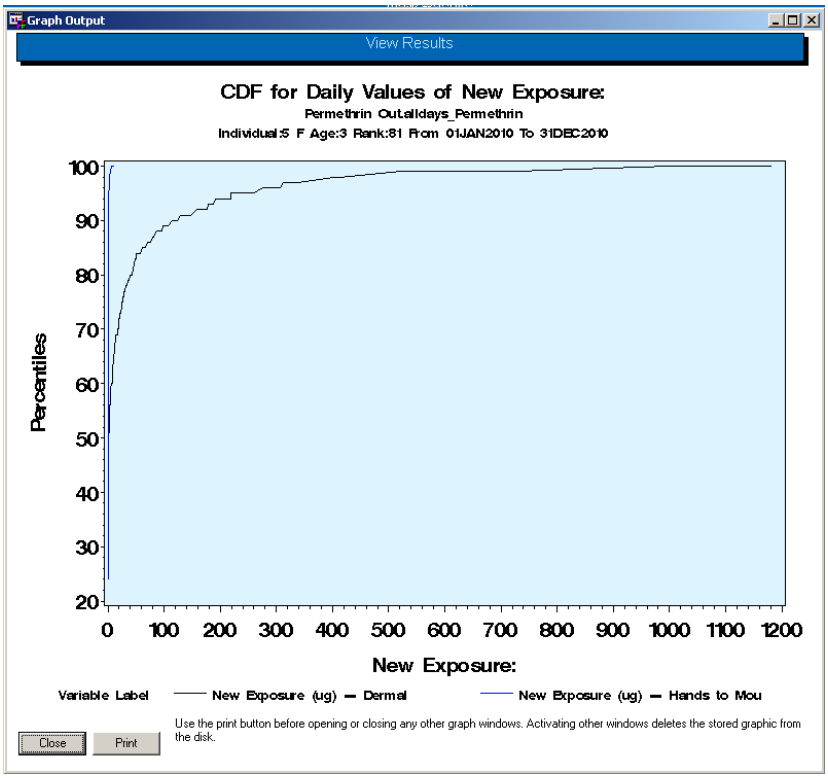
New Exposure:

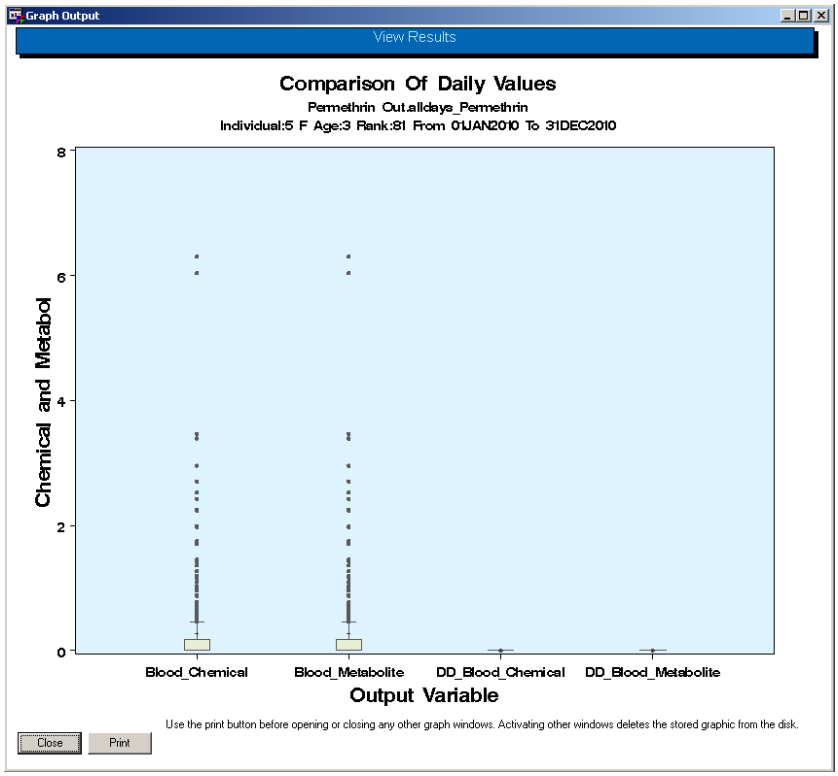
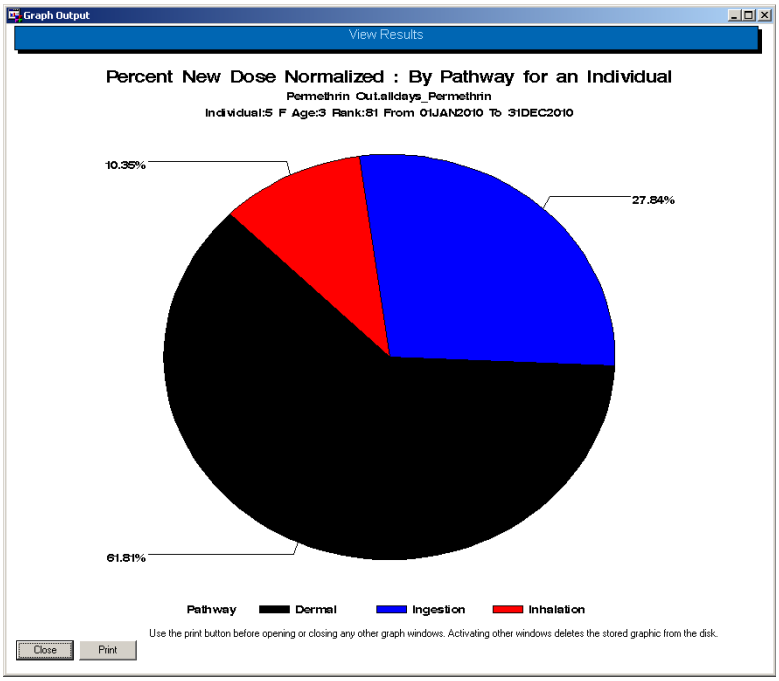
Permethrin N=500 out.persons_mean_Permethrin

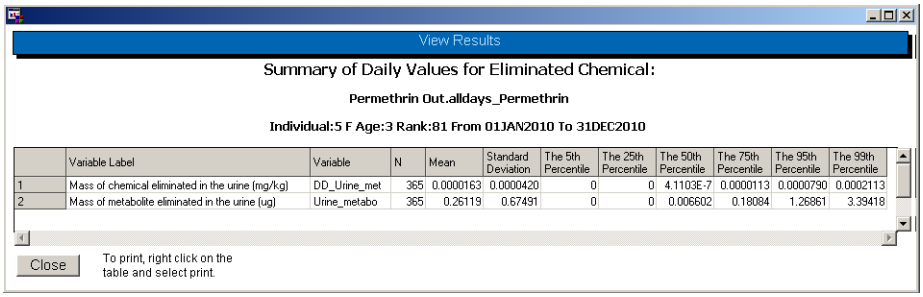
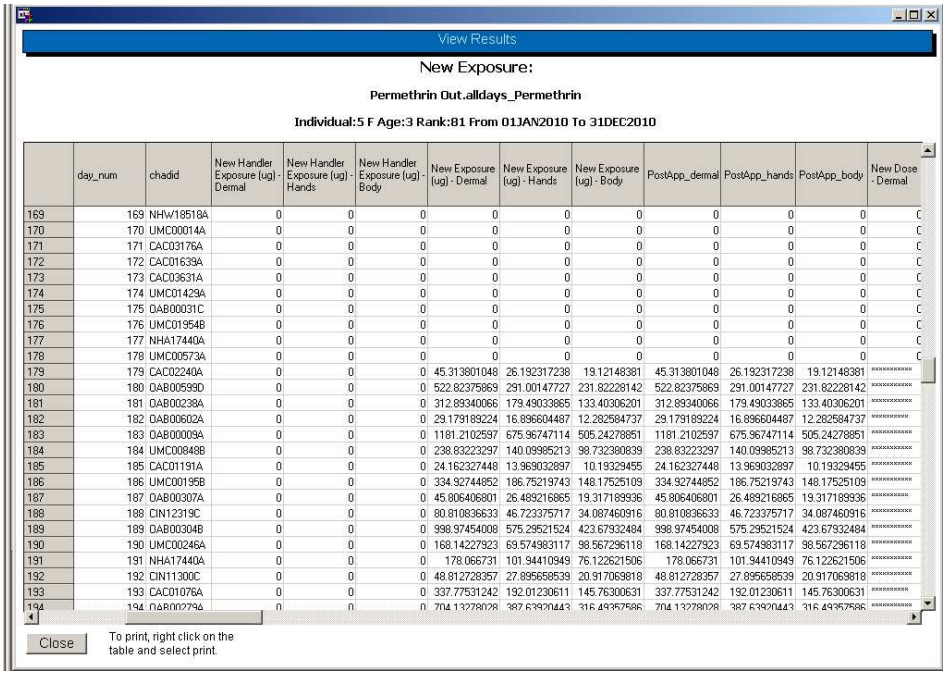
Selection: Males _Females Ages 3 to 5 Ranks 40 to 99

	Variable Label	Variable	N	Mean	Standard Deviation	The 5th Percentile	The 25th Percentile	The 50th Percentile	The 75th Percentile	The 95th Percentile	The 99th Percentile
1	New Exposure (ug) - Hands to Mouth	Expo_HTM	500	14.89746	55.05097	0	0	0	0	88.79809	221.00
2	New Exposure (ug) - Object to Mouth	Expo_OTM	500	0.76916	3.29971	0	0	0	0	4.18150	18.82971
3	New Exposure (ug) - Inhalation	Expo_Inhal	500	0.004456	0.01283	0	0	0	0	0.03466	0.06582
4	New Exposure (ug) - Body	Expo_body	500	23.05462	72.57244	0	0	0	0	161.03	410.68
5	New Exposure (ug) - Hands	Expo_hands	500	15.36187	43.51340	0	0	0	0	114.31	228.89
6	New Exposure (ug) - Dermal	Expo_dermal	500	38.41648	114.03	0	0	0	0	297.17	592.90

Select “Contribution By Pathway” as the output type. Select “New Exposure as” as the variable group and click <Display>. This creates the pie chart. Click<Close> to return to the previous screen.	
Click <Close> to return to the View Results screen. Click <View Results for an Individual>. Select person 5, or any other person with a higher ranking. Select “Time Series” as output type, “New Exposure” as variable group, and “Hands to Mouth” as the variable.	

Click <Display> to view the time series plot. Click <Close> to return to the previous screen.	
Select “CDF” as the output type. Select “New Exposure” as the variable group, highlight dermal and hand to mouth exposure, and click <Display>. This creates the CDF. Click<Close> to return to the previous screen.	

Select “Box and Whiskers” as the output type. Select “Chemical and Metabolite Entering Blood” as the variable group, highlight all the available variables, and click <Display>. This creates the box plot. Click<Close> to return to the previous screen.	
Select “Contribution by Pathway” as the output type. Select “New Dose Normalized to Body Mass” as the variable group and click <Display>. This creates the pie chart. Click<Close> to return to the previous screen.	

Select “Summary Table” as the output type. Select “Eliminated Chemical” as the variable group, highlight all variables, and click <Display>. This creates the table. Click<Close> to return to the previous screen.	
Select “Detailed Table” as the output type. Select “New Exposure” as the variable group, and click <Display>. This creates the table. You may need to page down to see the non-zero exposure estimates. Click <Close> to return to the previous screen.	

7 SHEDS-Residential: Batch Mode

The SHEDS model may also be run in batch mode. Runs in batch mode do not open any SAS windows. They are usually submitted via the Run dialog on the Start menu in Windows. Batch mode uses fewer computer resources, which may speed up long runs. This may be appropriate for overnight runs where the user has no need to view the progress of the job. Multiple batch jobs may be submitted at one time, also useful for overnight runs. Finally, sensitivity analysis or uncertainty analysis runs may also be conducted in batch mode, or by submitting the appropriate commands in a standard SAS session.

7.1 Installing Batch Capability

Along with the SAS program "Multimedia4.sas" and the default input files used by the interface, two additional files ("batch.sas" and "SHEDS.bat") are needed to run SHEDS-Residential in batch mode.

The file "batch.sas" does not require editing. Its contents are:

```
%Let comma = %index(%quote(&sysparm),%str(,));
%Let dir = %substr(%quote(&sysparm),1,%eval(&comma-1));
%Include "&dir\prg\multimedia4.sas";
%multimedia4(&sysparm);
```

The other file is "SHEDS.bat", **which must have its path names altered to match the SHEDS installation directory on the user's machine.** The default contents of "SHEDS.bat" are shown below.

```
"C:\Program Files\SAS64\SASFoundation\9.2\sas.exe"
"C:\SHEDS_Multimedia4\prg\batch.sas"
-sysparm "C:\SHEDS_Multimedia4,%1 %2 %3 %4 %5,64"
```

In the batch file, the three lines above should appear on a single line, as they are all part of the same command. The pathnames may need to be edited to conform to the user's computer. The first is the location of the sas.exe file itself. The second gives the location of the batch.sas program, which is usually in the \prg directory under the SHEDS-Residential installation directory. The third path (from the C: in the third line above, up to the comma) gives the location of the SHEDS installation directory. This file can be edited in any text editor.

7.2 Defining Inputs for a Batch Run

The main difficulty in submitting a SHEDS run is ensuring that all the necessary inputs are defined. This is a primary function of the interface itself. Hence, the easiest way to prepare a batch run is to define and save all the inputs using the interface. Inputs for several runs could be defined and saved without submitting any of these jobs. Alternatively, the user could prepare the

required input files using a standard SAS editor, but this places a greater burden on the user to ensure that all inputs have been supplied in a consistent manner.

Each set of inputs and settings is saved under a user-supplied job name. For example, suppose the user chooses the name “job1”. Whether defined through the interface or not, this requires the addition of a new record to the “runinfo” file found in the SHEDS installation directory, and new directories called “runs\job1\input” and “runs\job1\output” need to be created. Appropriate versions of the following SAS datasets must be defined for the run, either placed in the \input directory for the run or else found in the default data directory:

agegroups
areatreated
bwsa
chem_distributions
chemicals
cohorts
contactmedia
correlations
dates_fixed
dates_variable
diaryevents
diarylocs
diaryQArules
diaryquest
distributions
handlers
intervals
metsdists
metsmap
pop2000
scenarios
timeseries
variables

Even if the defaults are acceptable for all the above files, each job requires its own record in the RunInfo file. Either an existing record on the RunInfo file can be edited, or a new record added. Open the existing RunInfo file in the SAS editor, copy any record to a form a new record, and then hand-edit that new record. Alternatively, a new record may be added using SAS programming. For many users, these options can be performed more easily through the SHEDS graphical user interface (GUI). It is possible to prepare the RunInfo file using the GUI and then later submit the job in batch mode.

7.3 Submitting a Batch Run

To submit a SHEDS run in batch mode, use the Run dialog on the Windows Start menu. Enter the full path to the "batchrun.bat" file (with quotes needed if the path contains blanks or spaces), followed by a space and the name of the job to be run. For example,

```
"C:\SHEDS_Multimedia4\SHEDS.bat" job1
```

Do not quote the name of the job itself, even if it contains spaces. To submit the job "lawn and garden" (assuming that the "multimedia.bat" file is located in "C:\SHEDS_Multimedia4"), type

```
"C:\SHEDS_Multimedia4\SHEDS.bat" lawn and garden
```

and hit the return key to submit the commands.

A black DOS window should appear, along with another SAS window indicating the location of the source code, output, and log files. The file batch.log contains the information normally found in the SAS log window. The rest of the output from the run should be located in the \output directory under the job name.

7.4 Uncertainty and Sensitivity Runs

Uncertainty and sensitivity runs are submitted in exactly the same way as other batch runs. Note that these runs may take a long time to complete. A run of 200 populations of 1000 persons each takes the same time to complete as a variability-only run of 200,000 persons. This may take several days.

Uncertainty runs require extra input files for the "uncertainty clouds" that represent the possible parameter spaces for the uncertain inputs. These must be placed in the \input\unc folder under the location for the given run, or else in the data\unc folder under the SHEDS installation. The uncertainty clouds are in SAS data sets that must be prepared outside of SHEDS. However, the version 4 GUI allows the user to specify the file names for these clouds, and even allows the user to submit uncertainty runs.

The percentile scaling and Sobol's method of sensitivity analysis require special two-stage runs. However, these are submitted exactly like any other runs. Switches on the RunInfo file indicate the type of sensitivity analysis to be performed. Also, the variables input file will indicate which variables are being analyzed. The SHEDS GUI now handles these file edits and the submission of sensitivity runs, although the user may still submit them in batch mode.

Appendix A. Directories and Files

All of the directories that SHEDS-Residential uses are placed underneath the installation directory which is chosen by the user at install time. By default this is in the user's My Documents/Multimedia3.14 (or similar) directory. The install directory will be referred to as the install directory or <install> in the following discussion and diagrams.

A.1 Directories

The directories are laid out as follows on installation. The indentation of a directory name implies that it is within the directory above it.

<install>		
Data		
	Default	Default and constant input files
	Diet	Currently unused
Prg		SAS catalogs and macros implementing model
Runs		All input and output related to specific runs
	Permethrin Case Study	All input and output related to the example Permethrin Case Study
	Input	User edited files for run
	Output	Results for demonstration run
Setup		Files related to installation and un-installation

A.2 Critical Input Files

If using the interface, it is not necessary for the user to know where files are stored. For batch runs and advanced post-run analysis it becomes important. The table below shows where critical files are placed at installation or when a run is defined through the interface. All files in the Runs/<run name>/Input directory are modified by the interface (except the contactmedia.sas7bdat dataset). Additional input files (e.g., CHAD diaries) needed for runs can be found in the <install>/Data/Default/ directory.

<install>/		
	autoexec.sas	SAS start-up file. Many SAS options can be set here
	multimedia.bat	File used to run SHEDS in batch mode
	runinfo.sas7bdat	File containing run specific information generated by the interface
Runs/<run name>/Input/		

Required for Batch Runs	agegroups.sas7bdat	Defines age and genders to be used in simulation
	areatreated.sas7bdat	Fraction of area treated for indoor scenarios
	chemicals.sas7bdat	Chemicals present in the run
	chem_distributions.sas7bdat	Chemical specific variable distributions as defined for run
	scenarios.sas7bdat	Information for the application scenarios defined in the run
	correlations.sas7bdat	Correlation information
	cohorts.sas7bdat	Cohort information
	handlers.sas7bdat	Required for handler runs
	distributions.sas7bdat	Variable distributions as defined for run
	contactmedia.sas7bdat	List of contact media and their short names
One of These is Required	decay.sas7bdat	Decay and dispersion application information
	intervals.sas7bdat	Interval concentration information
	timeseries.sas7bdat	User defined time series concentrations for each media
One of These is Required	dates_variable.sas7bdat	Data required for model to determine stochastic application dates
	dates_fixed.sas7bdat	Data for user defined application dates

A.3 User Specified Output Files

The major output files for a typical variability run, their structure, and variable definitions are discussed in the SHEDS-Residential Technical Manual. Files related to sensitivity and uncertainty runs are discussed in the section on batch runs in this manual.

If a log file is specified by the user, on the Simulation Information screen, then it is put in <install>/Runs/<run name>/Output/saslog.txt. This file can be read in the SAS editor or any other editor of the user's choosing.

If a user requests a spreadsheet of inputs, on the Run screen, it will be placed in the installation directory and named after the run name: <install>/<run name>.xls. This file can be read from MS Excel 2003 or later.

A.4 Other Output Files

A.4.1 Diary Related Output Files

The number of available one-day activity diaries for each cohort and day type is listed in the file "diarycounts" in the \output directory for the given run.

A.5 Exporting SAS Datasets

To facilitate additional analyses in the software of your choosing, you may export data in a variety of formats. The export wizard can be accessed by selecting a dataset in SAS and then selecting Export Data from the main SAS File menu. For more information on the export wizard check the SAS help file index under "exporting data/Export Wizard for". To export data programmatically, use Proc Export. Again, information on specifics can be found in the SAS help files.

8 References

Glen G., Zartarian V.G., Smith, L., and Xue J. (2010). The Stochastic Human Exposure and Dose Simulation (SHEDS)-Residential Model Technical Manual. Prepared for the July 20-22, 2010 EPA FIFRA SAP, Crystal City, VA.

Isaacs K., Xue J., Stallings C., Zartarian V.G. (2010) Stochastic Human Exposure and Dose Simulation (SHEDS) Model for Multimedia, Multipathway Chemicals: Version 1 SHEDS-Dietary Module User Guide. Prepared for the July 20-22, 2010 EPA FIFRA SAP, Crystal City, VA.

Xue J. 2010. SHEDS-Dietary version 1.0 SAS code.

Xue J., Zartarian V.G., Nako S. (2010). The Stochastic Human Exposure and Dose Simulation (SHEDS)-Dietary Model Technical Manual. Prepared for the July 20-22, 2010 EPA FIFRA SAP, Crystal City, VA.

Appendix B. Reference Tables

B.1 Variable Names

Table B-1. Variable Names From Distributions File

Variable	Label	Units
Gender	Gender, M=male, F=female	[-]
Age	Age (full years)	years
Weight	Body weight	kg
DiaryT	Personal mean for DiaryKey ranking	[-]
DiaryA	Autocorrelation in diary ranks	[-]
DiaryNums	Pool selections for one-day diaries	[-]
DiaryReorder	Selections for diary re-ordering	[-]
Height	Height in cm	cm
BMR	Basal metabolic rate	megajoules/day
BVA	Basal alveolar ventilation rate	m3/day
Mets_max	Maximum allowed mets	mets
OxyDebt_max	Maximum allowed oxygen debt	(ml of O2)/kg
Slope_fast	Slope of fast anaerobic process	mets/min
Recovery	Recovery time for maximum debt	hr
p_Handler	Probability of being product handler	[-]
p_Lawn	Probability of having a lawn	[-]
p_Garden	Probability of having a vegetable garden	[-]
p_Pet	Probability of having a dog or cat	[-]
Area_House	Floor area of house	m2
Area_Lawn	Area of lawn to be treated	m2
Area_Garden	Area of garden to be treated	m2
Area_Pet	Surface area of pet to be treated	m2
f_Carpet	Fraction of indoor time on carpet	[-]
f_Lawn	Fraction of out-home time on lawn	[-]
f_Garden	Fraction of out-home time in garden	[-]
f_Pet	Fraction of time at home near pet	[-]
Background	Outdoor background concentration	ug/cm2
Dust_loading	Indoor dust loading on floor	ug/cm2
HouseNum	House number (for timeseries input)	[-]
HandWash_mean	Mean # of hand washings per day	1/day
v_BathDays	Vector for maximum # days between baths	days
v_ReEntry_in	Vector for indoor contact prohibition time	[-]
v_ReEntry_out	Vector for outdoor contact prohibition time	[-]
v_ReEntry_pet	Vector for pet contact prohibition time	[-]

v_TimeOfUse_in	Vector for indoor application hour	hr
v_TimeOfUse_out	Vector for outdoor application hour	hr
v_TimeOfUse_pet	Vector for hour of pet application	hr
f_AreaTreated	Fraction of house treated	[-]
f_Decay_in	Fraction lost per day indoors	1/day
f_Decay_out	Fraction lost per day outdoors	1/day
f_Decay_pet	Fraction lost per day on pet	1/day
f_UTratio	Untreated/treated ratio at Umax	[-]
Treated	Fraction of time in treated area	[-]
SurfaceType	Fraction of time on various surfaces	[-]
PetContact	Fraction of time around pet	[-]
Mets	Mets level for inhalation	mets
HandWash	Hand washing: 1=yes, 0=no	[-]
SoilIngest	Daily soil ingestion rate	mg/day
Dermal_Contact	Skin-Surface contact rate	1/hr
Dermal_TC	Surface-to-skin transfer coefficient	cm2/hr
Dermal_TE	Surface-to-skin transfer efficiency	[-]
Dermal_MaxLoad	Maximum Dermal Loading	ug/cm2
Dermal_Binding	Rate of penetration into skin surface	1/hr
Dermal_BrushOff	Fraction removed per hour by brush-off	1/hr
f_DermalHands	Fraction of dermal exposure on hands	[-]
f_Uncloth	Fraction of skin not clothed	[-]
f_HandMouth	Fraction of one hand that enters mouth	[-]
f_ObjFloor	Object-to-floor concentration ratio	[-]
Unit_Handler	Unit exposure during handling	ug/g
HandMouth_freq	Hand-mouthing events per hour	events/hr
HandMouth_TE	Removal efficiency during hand mouthing	[-]
ObjMouth_area	Object-mouth contact area	cm2
ObjMouth_freq	Object-mouthing events per hour	events/hr
ObjMouth_TE	Object-to-mouth transfer efficiency	[-]
f_RemovBath	Fraction removed during bath or shower	[-]
f_RemovHandWash	Fraction removed during hand washing	[-]
f_DermalBlood	Fraction absorbed from skin into blood	[-]
f_InhalBlood	Fraction absorbed from lungs into blood	[-]
f_IngestBlood	Fraction absorbed from GI tract into blood	[-]
f_Urine	Fraction of blood dose eliminated in urine	[-]
Freq_Lawn_Granul	Usage frequency for Lawn_Granul	[-]
Dates_Lawn_Granul	Usage dates for Lawn_Granul	[-]
Amount_Lawn_Granul	Amount used for Lawn_Granul	[-]
Freq_Lawn_Liquid	Usage frequency for Lawn_Liquid	[-]
Dates_Lawn_Liquid	Usage dates for Lawn_Liquid	[-]
Amount_Lawn_Liquid	Amount used for Lawn_Liquid	[-]
Freq_Veg_Powder	Usage frequency for Veg_Powder	[-]
Dates_Veg_Powder	Usage dates for Veg_Powder	[-]
Amount_Veg_Powder	Amount used for Veg_Powder	[-]
Freq_CC_Aerosol	Usage frequency for CC_Aerosol	[-]

Dates_CC_Aerosol	Usage dates for CC_Aerosol	[-]
Amount_CC_Aerosol	Amount used for CC_Aerosol	[-]
Freq_CC_Liquid	Usage frequency for CC_Liquid	[-]
Dates_CC_Liquid	Usage dates for CC_Liquid	[-]
Amount_CC_Liquid	Amount used for CC_Liquid	[-]
Freq_Ind_FIK	Usage frequency for Ind_FIK	[-]
Dates_Ind_FIK	Usage dates for Ind_FIK	[-]
Amount_Ind_FIK	Amount used for Ind_FIK	[-]
Freq_Ind_Fogger	Usage frequency for Ind_Fogger	[-]
Dates_Ind_Fogger	Usage dates for Ind_Fogger	[-]
Amount_Ind_Fogger	Amount used for Ind_Fogger	[-]
Freq_Pet_Spot	Usage frequency for Pet_Spot	[-]
Dates_Pet_Spot	Usage dates for Pet_Spot	[-]
Amount_Pet_Spot	Amount used for Pet_Spot	[-]
Freq_Pet_Liquid	Usage frequency for Pet_Liquid	[-]
Dates_Pet_Liquid	Usage dates for Pet_Liquid	[-]
Amount_Pet_Liquid	Amount used for Pet_Liquid	[-]

Appendix C. Probability Density Functions

The explicit probability density functions (pdf's) utilized by SHEDS are listed below. Note that some of these may have alternate parametrizations, so the user must be careful when obtaining distributions from the literature. The expressions "Exp," "Sqrt," "Log," and "Γ" refer to the exponential, square root, natural logarithm, and gamma functions, respectively.

C.1 Beta

The beta distribution in SHEDS has a lower bound of zero, an upper bound of one, and two shape parameters v1 and v2. The restrictions are v1>0 and v2>0. When v1< v2 then the mean is below ½ and the distribution is positively skewed, whereas when v1 > v2 the mean is above ½ and the distribution is negatively skewed. For v1=v2 the mean is at ½ and the shape is symmetric. The PDF is

Equation E-1

$$p(x) = x^{v1-1} (1-x)^{v2-1} \Gamma(v1+v2) / (\Gamma(v1) \Gamma(v2)), \text{ for } 0<x<1$$

Here 'Γ' is the mathematical gamma function, not the gamma distribution. The gamma function is a generalization of the factorial function to non-integer arguments; for integers, Γ(1+n) = n!. The beta is a useful form for variables known to be bounded, due to the wide variety of shapes that it can have. For v1>1 and v2>1, the PDF of the beta has a single peak, away from the bounds. When 0<v1<=1, the PDF is large near zero, and when 0<v2<=1, it is large near one. These properties allow the beta to have the so-called 'J' or 'U' shapes. The mean of a beta distribution is at $\mu = v1 / (v1+v2)$, and the standard deviation is $\sigma = Sqrt[v1\ v2 / (v1+v2+1)] / (v1+v2)$. If one wishes to construct a beta with a given mean μ and standard deviation σ, then choose $v1 = (\mu^2-\mu^3)/\sigma^2 -\mu$, and $v2 = v1 (1-\mu) /\mu$. This will only be possible if $0<\mu<1$ and $\sigma^2 < \mu (1-\mu) \leq 1/4$.

C.2 Exponential

The exponential in SHEDS has two parameters, the minimum (v1) and the mean (v2), with the restriction that v1 < v2. Some users may be more familiar with a single parameter exponential distribution, which has a minimum of zero and is characterized by a decay rate constant. The SHEDS exponential is similar, apart from a shift of v1 units to the right. The decay rate of the SHEDS exponential is given by 1/(v2-v1). The standard deviation of an exponential is (v2-v1). If the user wants an exponential with a half-life τ, then set v2 = v1+ τ / Log[2] . The PDF of the SHEDS exponential is

Equation E-2

$$p(x) = Exp[-(x-v1)/(v2-v1)] / (v2-v1), \quad \text{for } x>v1$$

C.3 Gamma

The gamma distribution in SHEDS is bounded below by zero and has two parameters, the shape parameter v1 and the scale parameter v2. The restrictions are v1>0 and v2>0. The shape parameter v1 controls the appearance of the PDF. Shape parameters less than one lead to a monotonically decreasing form with the highest probability at zero. If v1=1, then the gamma is identical to an exponential that starts

at zero and has a mean given by the gamma parameter v1. If v1>1, then the gamma somewhat resembles the lognormal, rising from zero to a peak probability, and then gradually declining with an overall positive skewness. The mean of the gamma is at μ = v1 v2, and the standard deviation is σ = v2 Sqrt(v1). The PDF of the SHEDS gamma is

Equation E-3

$$p(x) = v2^{-v1}\, x^{v1-1}\, \mathrm{Exp}(-x/v2) / \Gamma(v1), \quad \text{for } x>0$$

C.4 Lognormal

The lognormal in SHEDS is bounded below by zero and has two parameters, the geometric mean GM (v1) and the geometric standard deviation GSD (v2). The restrictions are v1>0 and v2>1. Many variables in exposure science are approximately lognormally distributed, so its use is fairly common. If a variable 'x' has a lognormal distribution, then log(x) has a normal distribution.

The geometric mean (GM) of a lognormal distribution is also its median. Log(GM) is the mean of the distribution of log(x). Log(GSD) is the standard deviation of log(x). Since standard deviations must be positive, then Log(GSD)>0, which implies GSD>1. The PDF of the SHEDS lognormal is

Equation E-4

$$p(x) = \mathrm{Exp}[(-1/2)\,(\mathrm{Log}[x/v1] / \mathrm{Log}[v2])^2\,] / (x\ \mathrm{Sqrt}[2\,\pi\,]\ \mathrm{Log}[v2]\,), \quad \text{for } x>0$$

If GM and GSD are given, then the lognormal has arithmetic mean and standard deviation

Equation E-5

$$\mu = \mathrm{GM}\ \mathrm{Exp}[(1/2)\,(\mathrm{Log}(\mathrm{GSD}))^2\,],$$
$$\sigma = \mathrm{GM}\ \mathrm{Sqrt}[\mathrm{Exp}(\,[\mathrm{Log}(\mathrm{GSD})]^2)\ (\mathrm{Exp}(\,[\mathrm{Log}(\mathrm{GSD})]^2)-1)].$$

If the user knows the arithmetic mean μ and arithmetic standard deviation σ of the lognormal instead of the GM and GSD, then these can be converted as follows:

Equation E-6

$$\mathrm{GM} = \mu\ /\ \mathrm{Sqrt}(1 + \sigma^2/\mu^2),$$
$$\mathrm{GSD} = \mathrm{Exp}(\mathrm{Sqrt}(\mathrm{Log}(1 + \sigma^2/\mu^2))).$$

If instead, one has the mean μ_{log} and standard deviation σ_{log} of log(x), then use

Equation E-7

$$\mathrm{GM} = \mathrm{Exp}(\mu_{log}),$$
$$\mathrm{GSD} = \mathrm{Exp}(\sigma_{log}).$$

C.5 Normal

This is the normal or Gaussian distribution commonly used in statistics. The normal has two parameters: the mean (v1) and the standard deviation (v2), with v2>0. Note that the normal is unbounded, so it is a good idea to provide lower and upper truncation points to prevent physically impossible values from being returned. The PDF of the normal is

Equation E-8

$$p(x) = \text{Exp}[-(x-v1)^2/(2\ v2^2)] / (\text{Sqrt}[2\ \pi]\ v2)$$

C.6 Point

A point value means that the same value is always returned. This is sometimes called a *fixed* or *constant* form. The point has one numeric argument (v1) which is the value that is to be returned. The mean is v1 and the standard deviation is zero. The sampling frequency does not matter for points. While points are technically discrete, here they are classified with the continuous distributions since they are applied to variables that are expected to reside on a continuous scale, but happen to be assigned no variability.

C.7 Triangular

The triangular distribution has a probability density function (PDF) that is shaped like a triangle. The three parameters locate the vertices, with v1=minimum, v2=peak, v3=maximum. The restrictions are v1<= v2 <= v3, with v1<v3. The mean value of this distribution is located at $\mu = (v1+v2+v3)/3$, which coincides with the peak only when v2 is midway between v1 and v3. The standard deviation is $\sigma = \text{Sqrt}[(v1^2+v2^2+v3^2-v1v2-v1v3-v2v3)/18]$. It is possible for the peak to be located at either extreme, forming a right triangle. The PDF of the triangular is

Equation E-9

$$p(x) = 2\ (x-v1) / [(v2-v1)\ (v3-v1)], \quad \text{for } v1 \le x \le v2$$
$$= 2\ (v3-x) / [(v3-v2)\ (v3-v1)], \quad \text{for } v2 \le x \le v3$$

C.8 Uniform

The uniform is characterized by two parameters, the minimum (v1) and the maximum (v2), with v1<v2. All values between v1 and v2 are equally likely to be returned. The mean is $\mu = (v1+v2)/2$ and the standard deviation is $\sigma = (v2-v1) / \text{Sqrt}(12)$. The PDF of the uniform is

Equation E-10

$$p(x) = 1 / (v2-v1), \quad \text{for } v1 < x < v2.$$

C.9 Weibull

The Weibull distribution in SHEDS is bounded below by zero and has two parameters, the shape parameter v1 and the scale parameter v2. The restrictions are v1>0 and v2>0. The Weibull has slightly different properties from a gamma, but there is a strong overall resemblance. When the shape parameter $v1 \le 1$, the Weibull is monotonically decreasing. For v1=1, it reduces to an exponential. For v1>1, it rises to a peak and then declines gradually in a long tail. The mean is $\mu = v2\ \Gamma(1+1/v1)$, and the standard deviation is $\sigma = v2\ \text{Sqrt}[\Gamma(1+2/v1) - (\Gamma(1+1/v1))^2]$. Here '$\Gamma$' is the mathematical gamma function, not

the gamma distribution. The gamma function is a generalization of the factorial function to non-integer arguments; for integers, $\Gamma(1+n) = n!$. The PDF of the Weibull distribution is

Equation E-11

$$p(x) = v1\ v2^{-v1}\ x^{v1-1}\ \text{Exp}\ [-(x/v2)^{v1}], \quad \text{for } x>0.$$

C.10 Binomial Distributions

Binomial distributions have only two possible outcomes, for example, the outcome of yes/no tests. The usual statistical notation would be (p_1, p_2), where p_1 and p_2 are between 0 and 1 and sum to 1. However, the SHEDS code implements binomial distributions by having the user specify only the probability of a "yes". The probability of "no" is implied by 1 - "yes".

C.11 Discrete Probability Density Functions

Multinomial variables allow more than two possible outcomes. The usual statistical notation would be $(p_1, p_2, \ldots, p_n)$, where each p_i is between 0 and 1 and the p_i's sum to 1. In SHEDS, multinomial variables are called probability vectors. The user must supply the entire set of probabilities.